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(54) **LIQUID CRYSTAL COMPOUND, AND LIQUID CRYSTAL DISPLAY**

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(51) **Int. Cl.**

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C09K 19/20	(2006.01)
C09K 19/12	(2006.01)
C07C 69/76	(2006.01)
C07C 25/24	(2006.01)
C07C 43/225	(2006.01)

(52) **U.S. Cl.**

USPC **428/1.1**; 252/299.01; 252/299.64; 252/299.67; 560/65; 570/127; 570/128

(58) **Field of Classification Search**

CPC C09K 19/3048; C09K 19/3059; C09K 19/3066; C09K 19/3086; C09K 2019/2007; C09K 2019/2014; C09K 2019/0466

USPC 570/127, 128; 252/299.64, 299.67; 428/1.1; 560/65

See application file for complete search history.

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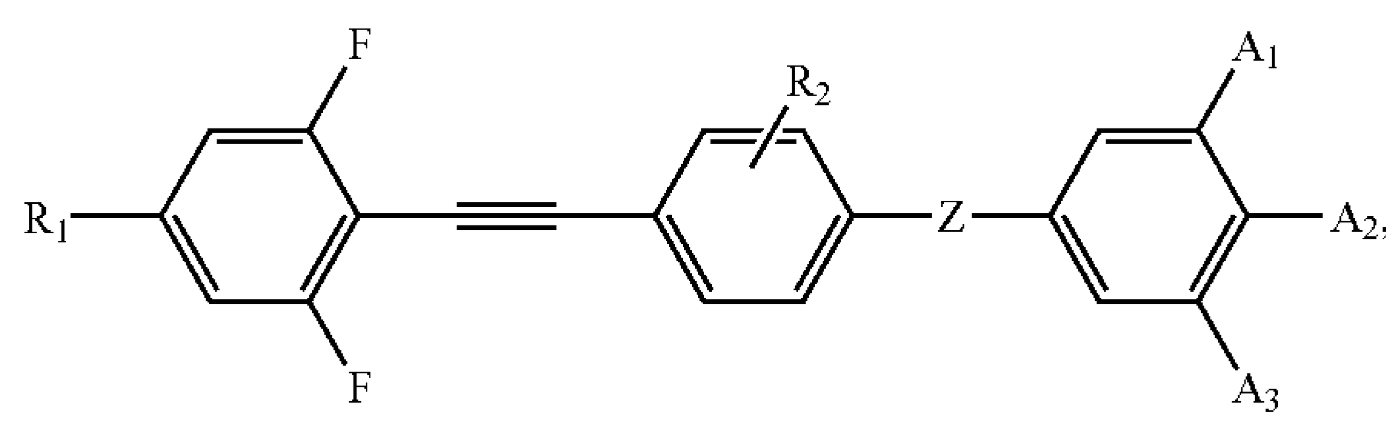
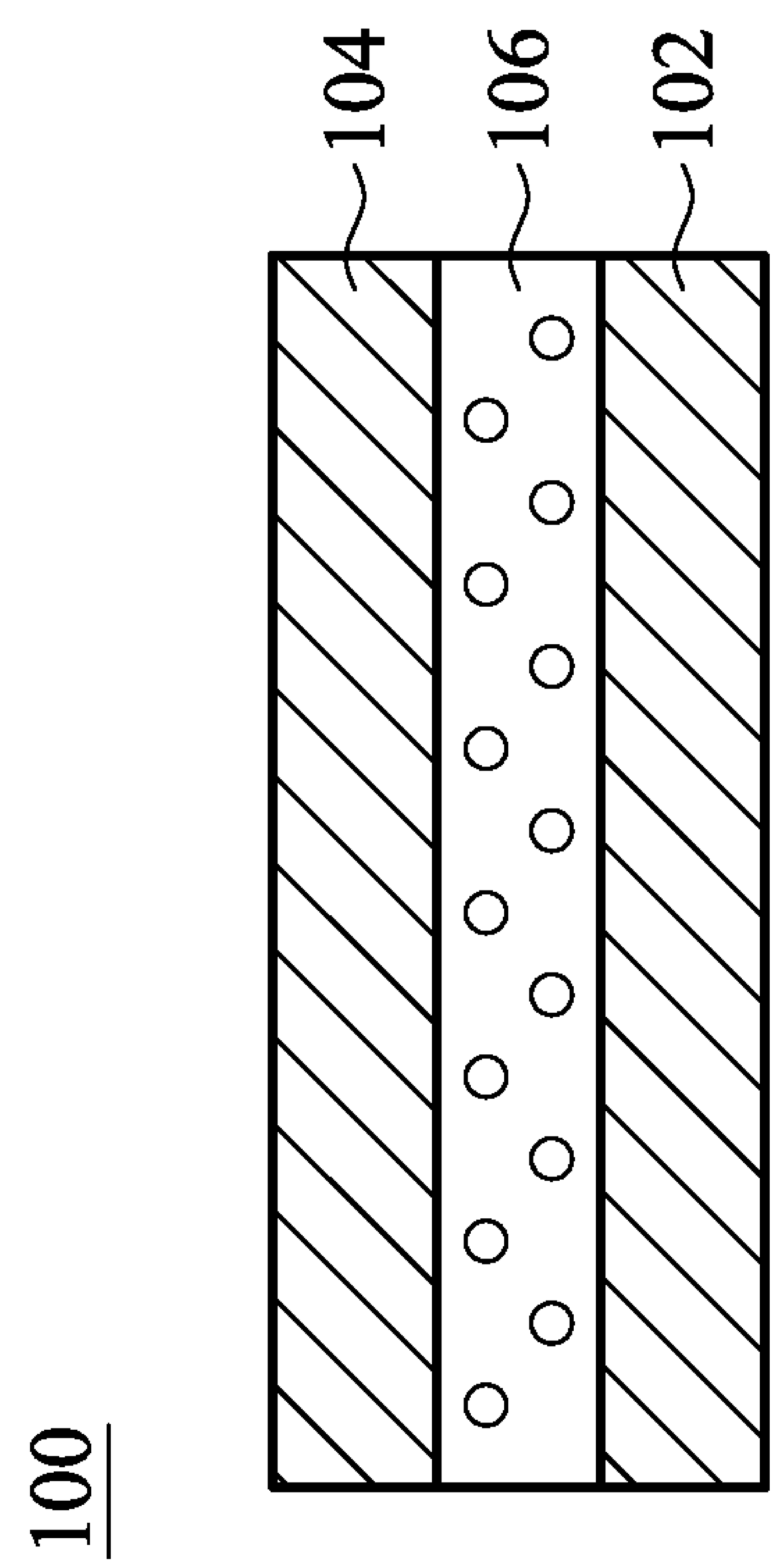
(57) **ABSTRACT**

An embodiment of the invention provides a liquid crystal compound having the following formula:



wherein A_1, A_2, and A_3 are independently hydrogen, halogen, cyano, thiocyanato, or —OCF_3; R_1 is hydrogen, halogen, C_1-C_{12} alkyl, C_1-C_{12} alkoxy, C_1-C_{12} haloalkyl, C_2-C_{12} alkenyl, or C_2-C_{12} alkynyl; R_2 is hydrogen, halogen, C_1-C_6 alkyl, C_1-C_6 haloalkyl, cyano, or —OCF_3; and Z is —O—, —CH_2O—, —C(O)O—, —OCO—, —C(O)NH—, —CH═CH—, or —C≡C—. In another embodiment, a liquid crystal display including the liquid crystal compound is also provided.

13 Claims, 1 Drawing Sheet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106
102
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LIQUID CRYSTAL COMPOUND, AND LIQUID CRYSTAL DISPLAY

CROSS REFERENCE TO RELATED APPLICATIONS

This Application claims priority of Taiwan Patent Application No. 100138436, filed on Oct. 24, 2011, the entirety of which is incorporated by reference herein.

BACKGROUND OF THE DISCLOSURE

1. Field of the Invention

The present invention relates to a liquid crystal compound, and in particular relates to a liquid crystal compound having high dielectric anisotropy.

2. Description of the Related Art

As technology has rapidly developed, various portable electronic products such as mobile phones, laptops, digital cameras, PDA, MP3, MP4, and etc. have become very important in modern day life. Meanwhile, advantages of liquid crystal displays include a small-size, light-weight, and low electricity consumption, and thus they have been frequently used in recent years. In a liquid crystal display, a liquid crystal material, which will affect the performance of a device using the same, plays an important role in the development of liquid crystal displays.

A good liquid crystal material should be, for example, stable toward water, air, heat, and light and have an appropriate dielectric anisotropy ($\Delta\in$), birefringence (Δn), and elastic constant (K_{ii}). An appropriate liquid crystal material can be chosen depending on particular requirements of liquid crystal displays.

Dielectric anisotropy ($\Delta\in$) refers to the difference between a dielectric coefficient in a parallel direction ($\in$//)O and a dielectric coefficient in a vertical direction ($\in\perp$). In other words, $\Delta\in=\in//-\in\perp$. Therefore, when $\in//>\in\perp$, it is called a positive diamagnetic anisotropy liquid crystal. When $\in//<\in\perp$, it is called a negative diamagnetic anisotropy liquid crystal. The value (positive or negative) of the diamagnetic anisotropy determines whether the liquid crystal is parallel or vertical to the electric field and whether light will pass through the liquid crystal layer or not. In addition, the diamagnetic anisotropy of a liquid crystal and driving voltage can be presented by the following formula:

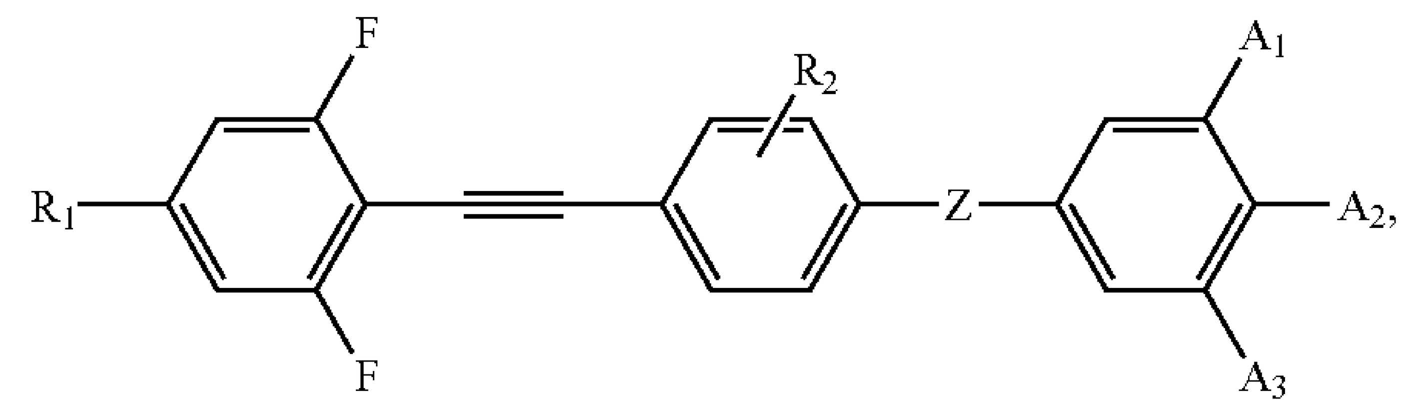
$$V_{th} = \pi\left(\frac{K_{ii}}{\Delta\varepsilon}\right)^{1/2}$$

The larger the diamagnetic anisotropy, the lower the driving voltage. Therefore, the liquid crystal display having high diamagnetic anisotropy can work with a lower voltage. However, diamagnetic anisotropies of most liquid crystal materials are smaller than 3.5, which is not satisfactory for modern day liquid crystal display use.

Therefore, a liquid crystal material having high diamagnetic anisotropy is desirable to decrease driving voltage.

BRIEF SUMMARY OF THE DISCLOSURE

An embodiment of the invention provides a liquid crystal compound having the following formula:



wherein A_1, A_2, and A_3 are independently hydrogen, halogen, cyano, thiocyanato, or —OCF_3; R_1 is hydrogen, halogen, C_1-C_{12} alkyl, C_1-C_{12} alkoxy, C_1-C_{12} haloalkyl, C_2-C_{12} alkenyl, or C_2-C_{12} alkynyl; R_2 is hydrogen, halogen, C_1-C_6 alkyl, C_1-C_6 haloalkyl, cyano, or —OCF_3; and Z is —O—, —CH_2O—, —C(O)O—, —OCO—, —C(O)NH—, —CH═CH—, or —C≡C—.

Another embodiment of the invention provides a liquid crystal display, comprising: a first substrate; a second substrate disposed opposite to the first substrate; and a liquid crystal layer disposed between the first substrate and the second substrate, wherein the liquid crystal layer comprises the above described liquid crystal compound.

A detailed description is given in the following embodiments with reference to the accompanying drawings.

BRIEF DESCRIPTION OF THE DRAWINGS

The present invention can be more fully understood by reading the subsequent detailed description and examples with references made to the accompanying drawings, wherein:

FIG. **1** is cross section of a liquid crystal display according to one embodiment of the invention.

DETAILED DESCRIPTION OF THE DISCLOSURE

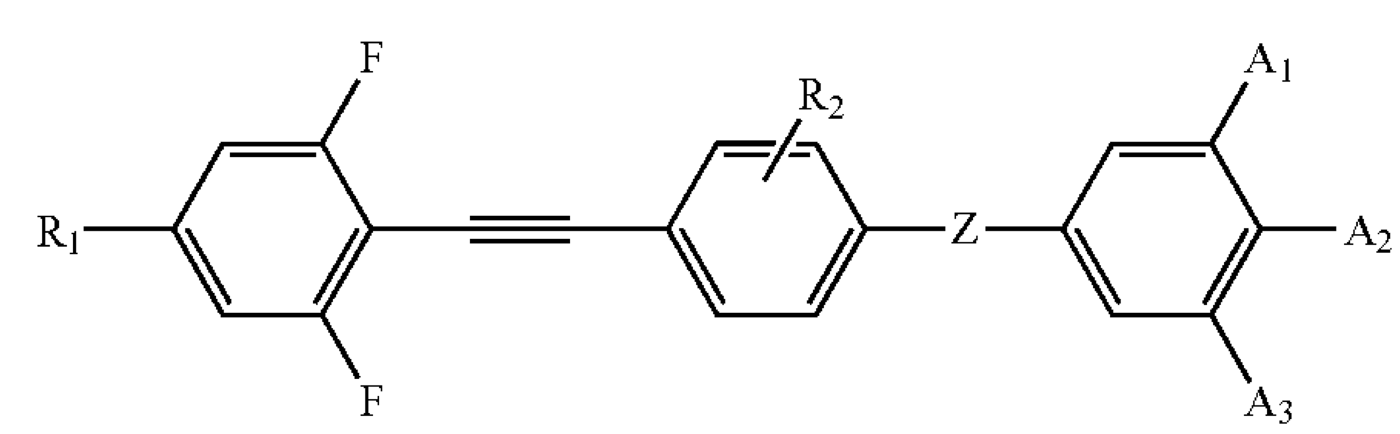
The following description is of the best-contemplated mode of carrying out the invention. This description is made for the purpose of illustrating the general principles of the invention and should not be taken in a limiting sense. The scope of the invention is best determined by reference to the appended claims.

Moreover, the formation of a first feature over and on a second feature in the description that follows may include embodiments in which the first and second features are formed in direct contact, and may also include embodiments in which additional features may be formed between the first and second features, such that the first and second features may not be in direct contact.

In one embodiment, a liquid crystal compound having high diamagnetic anisotropy is provided, wherein a driving voltage of a liquid crystal display can be decreased when the liquid crystal compound is added into the liquid crystal formulation.

A liquid crystal compound may have following formula:

(I)

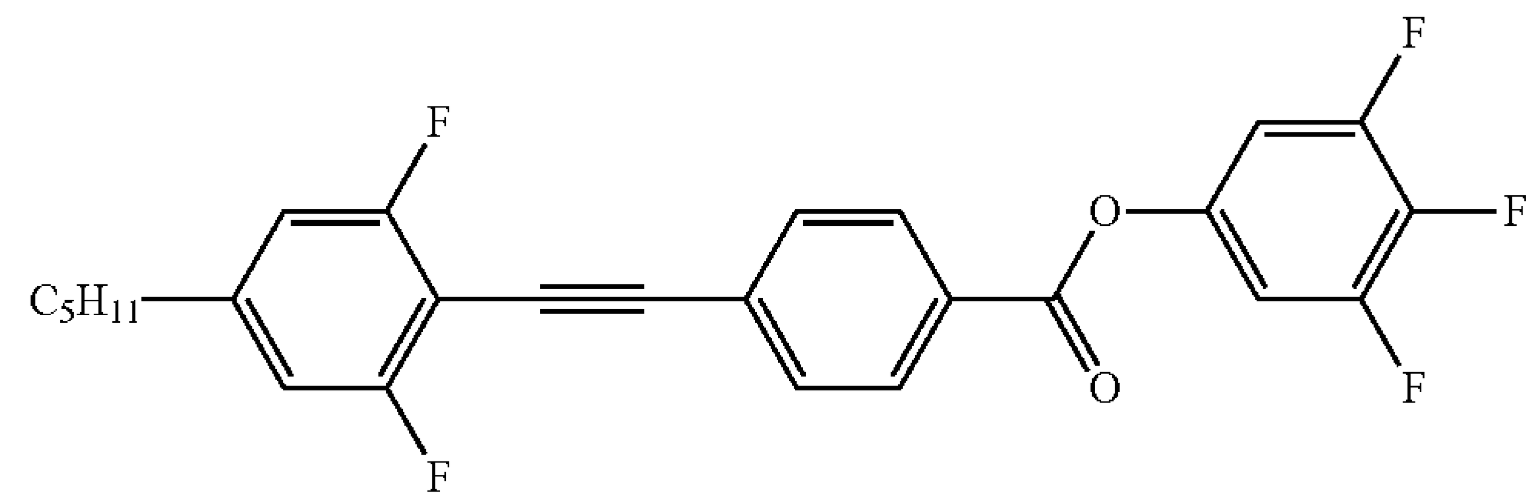


wherein A_1, A_2, and A_3 are independently hydrogen, halogen, cyano, thiocyanato, or —OCF_3; R_1 is hydrogen, halogen, C_1-C_{12} alkyl, C_1-C_{12} alkoxy, C_1-C_{12} haloalkyl, C_2-C_{12} alkenyl, or C_2-C_{12} alkynyl; R_2 is hydrogen, halogen, C_1-C_6 alkyl, C_1-C_6 haloalkyl, cyano, or —OCF_3; and Z is —O—, —CH_2O—, —C(O)O—, —OCO—, —C(O)NH—, —CH═CH—, or —C≡C—. The liquid crystal compound may have high diamagnetic anisotropy. For example, the diamagnetic anisotropy is above 45. For example, the diamagnetic anisotropy is between 45 and 85. In one embodiment, A_1, A_2, and A_3 are independently halogen or cyano. In another embodiment, R_1 is C_1-C_{12} alkyl or C_1-C_{12} alkoxy. In still another embodiment, R_2 is hydrogen. In still another embodiment, Z is —C(O)O— or —C(O)NH—.

Table 1 presents specific examples of the liquid crystal compound (I). However, these are, of course, merely examples and are not intended to be limiting.

TABLE 1

1



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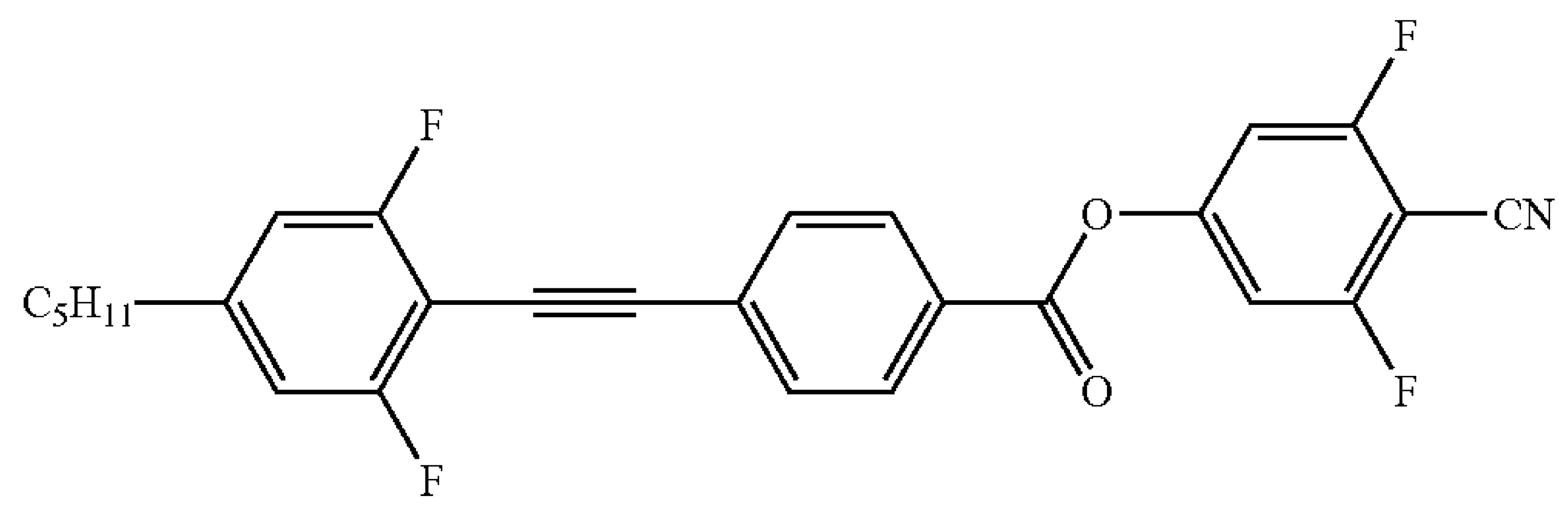

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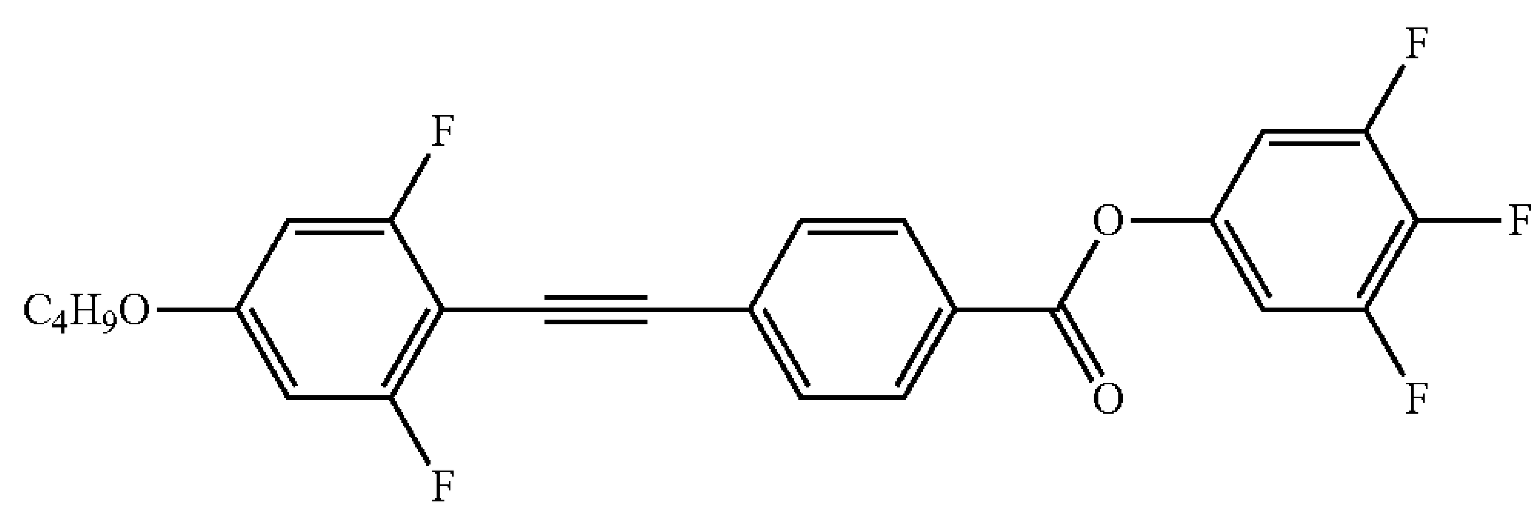

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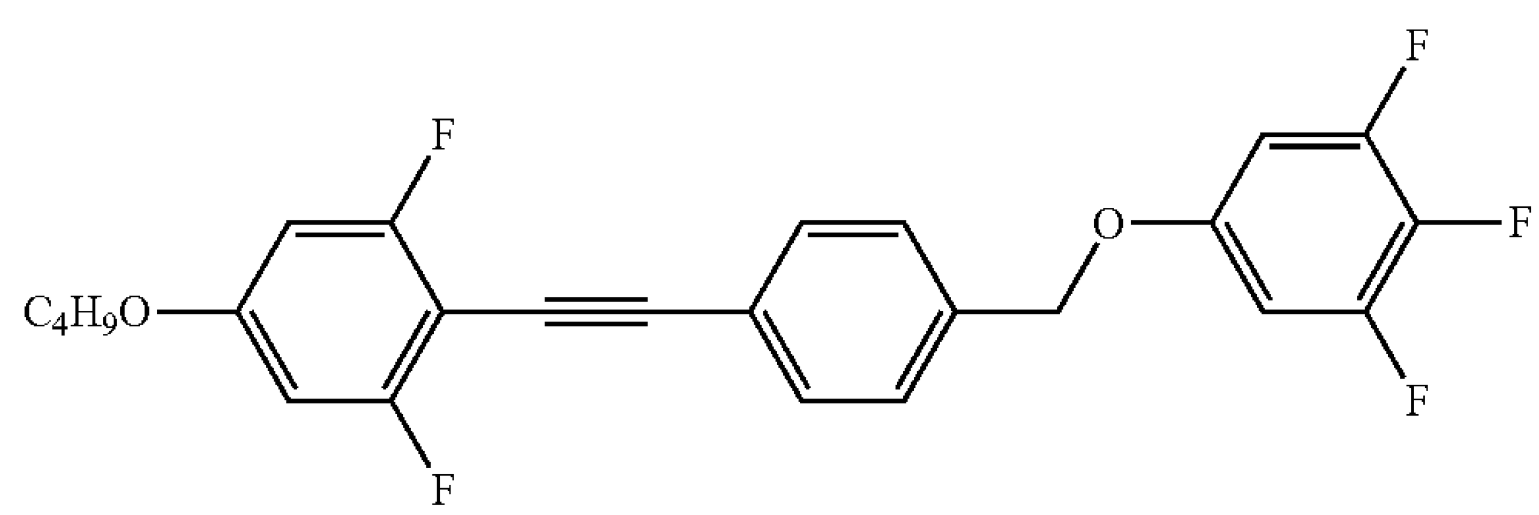

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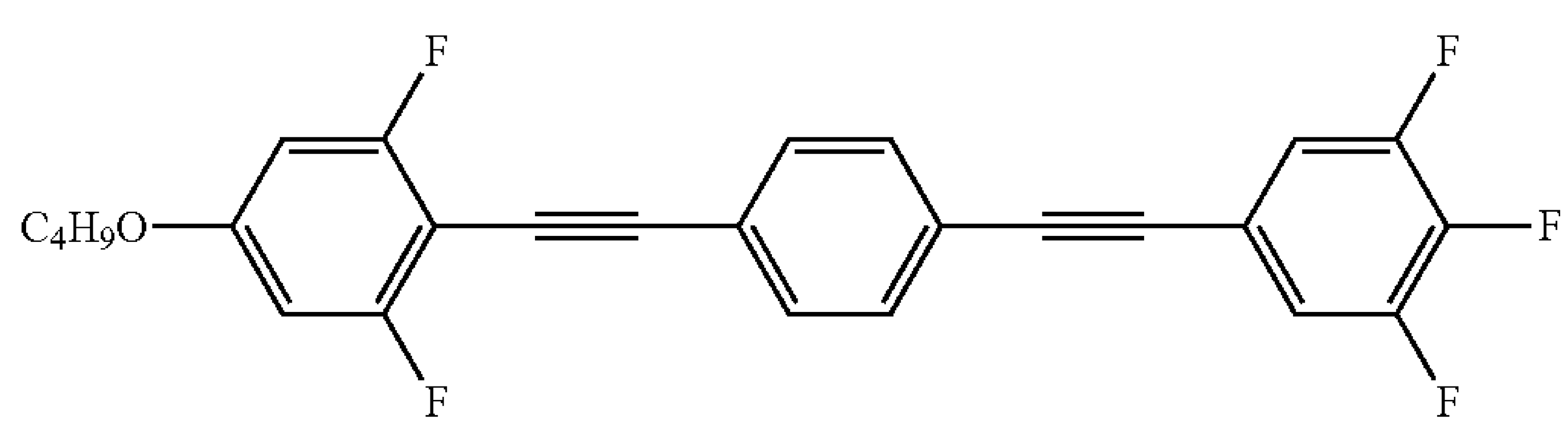

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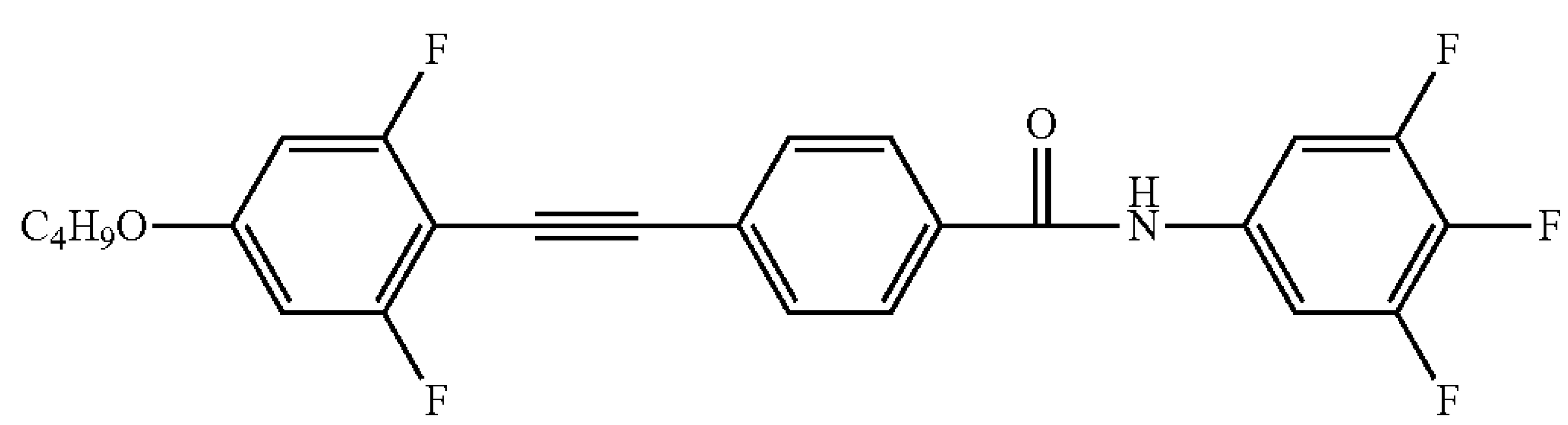

TABLE 1-continued

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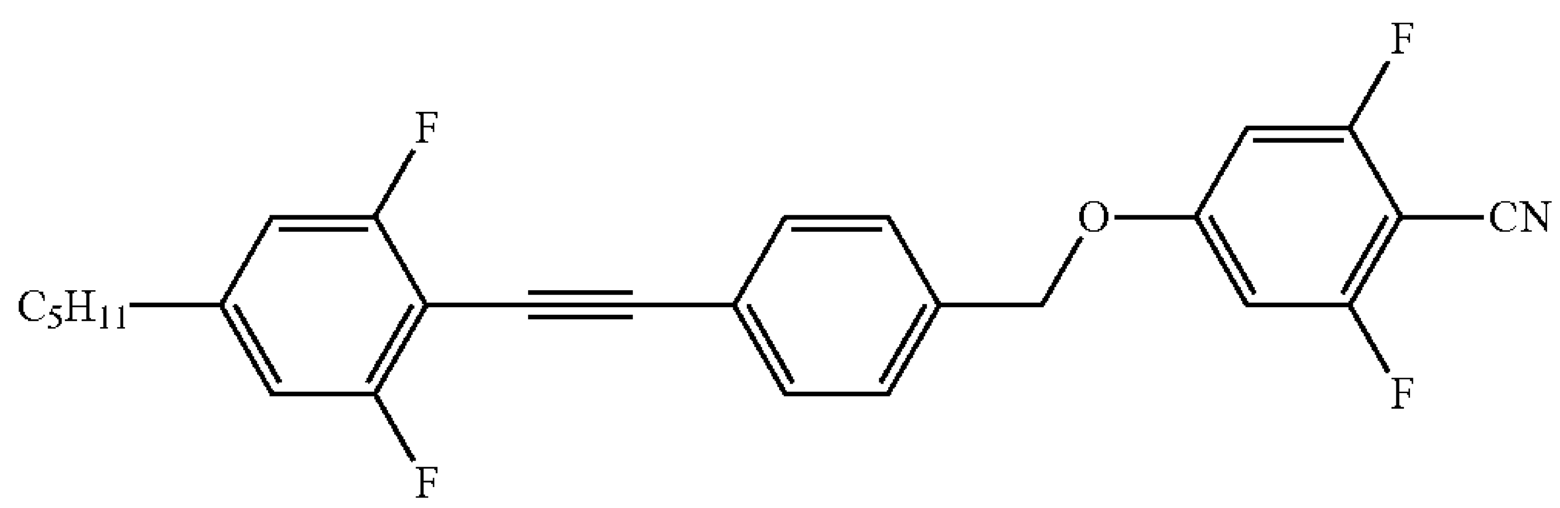

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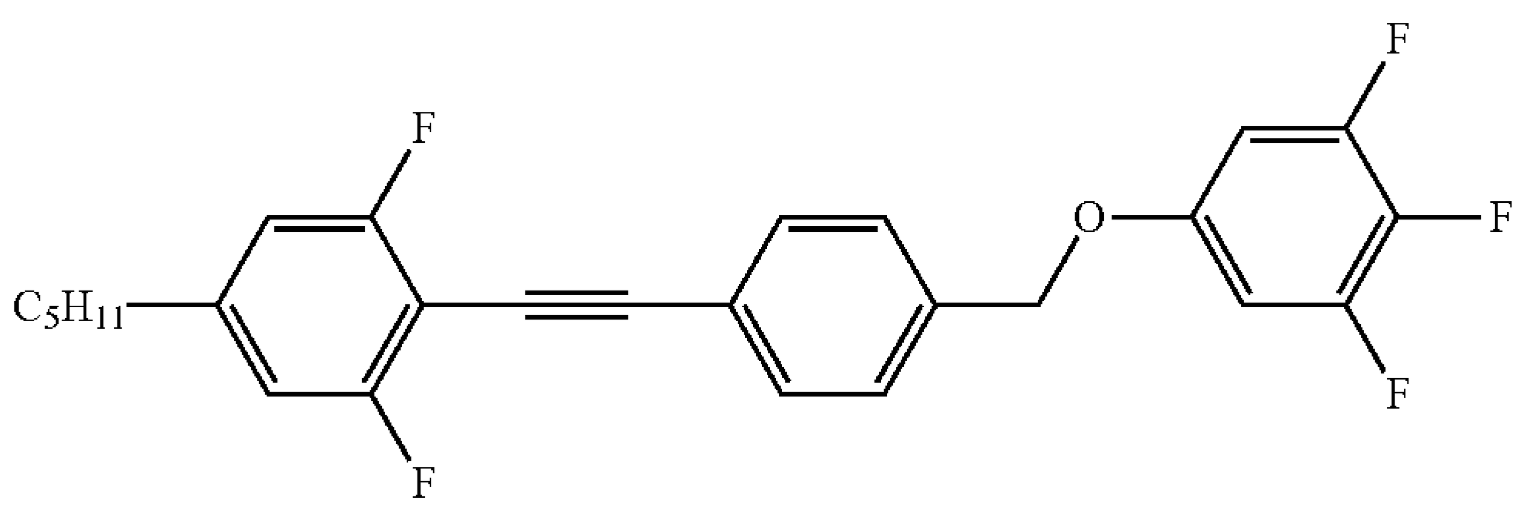

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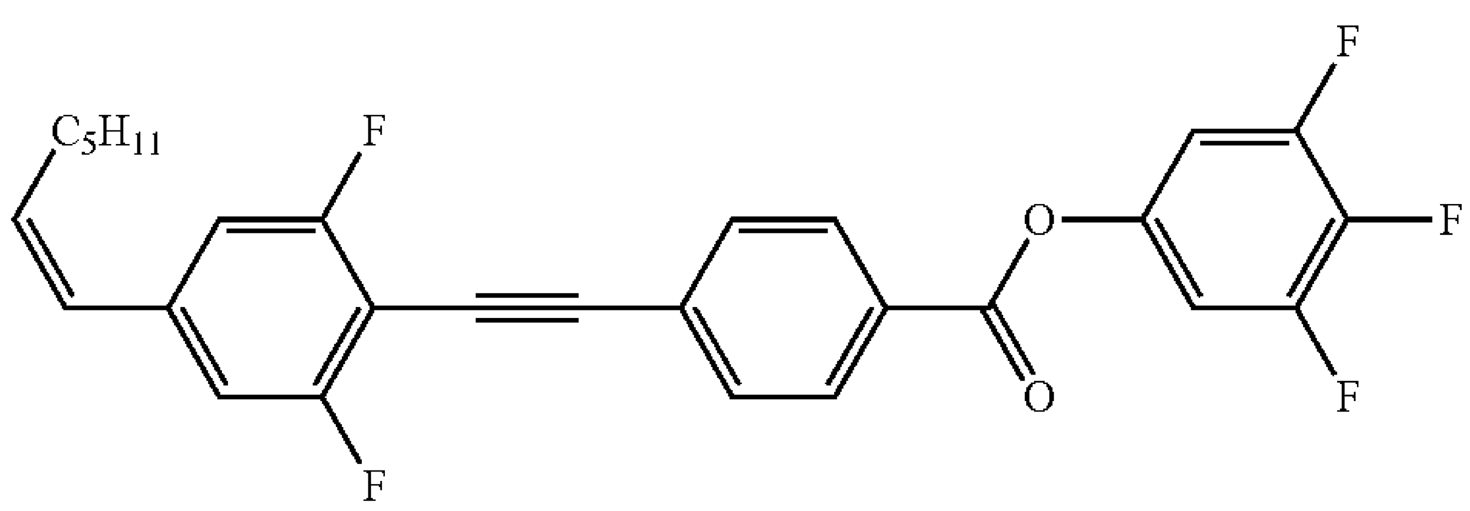

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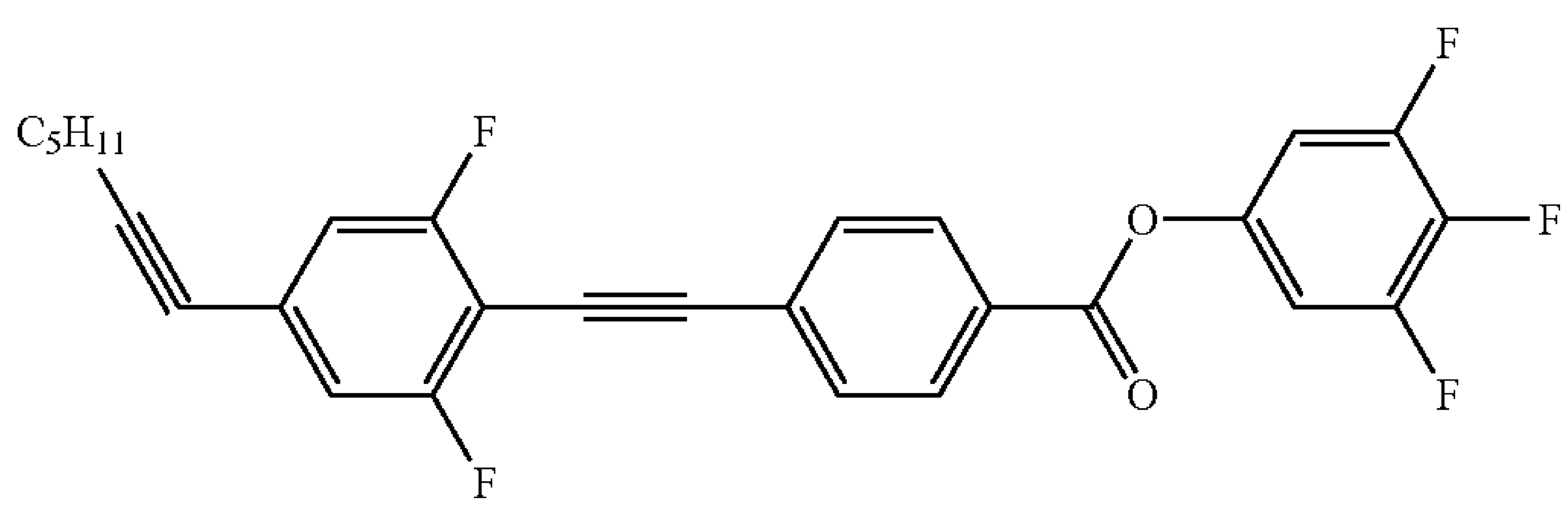

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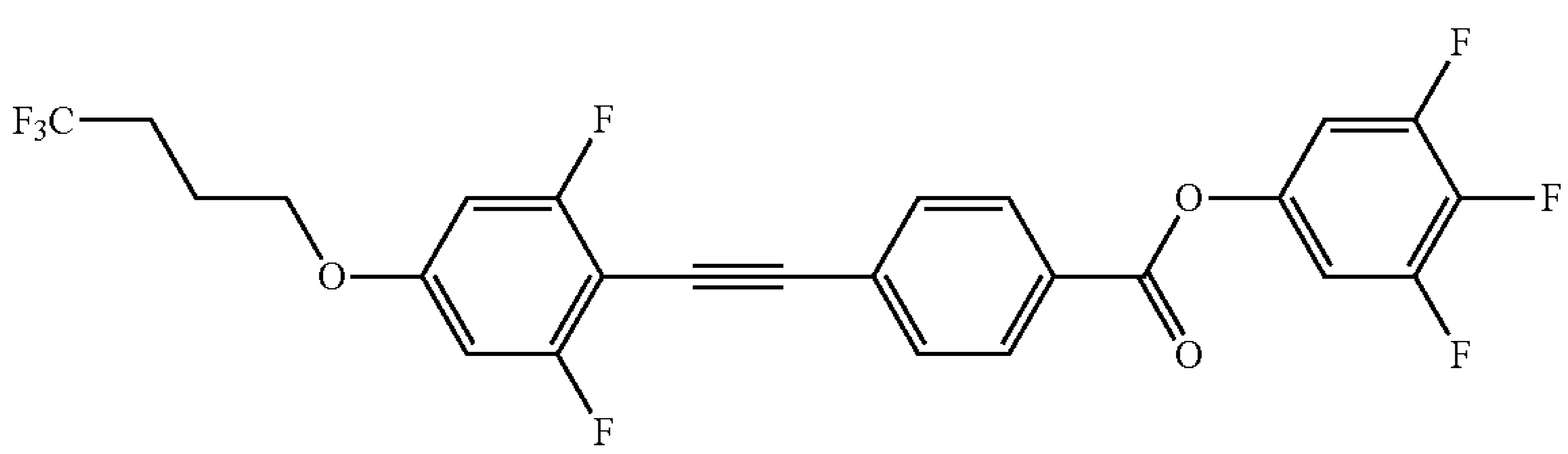

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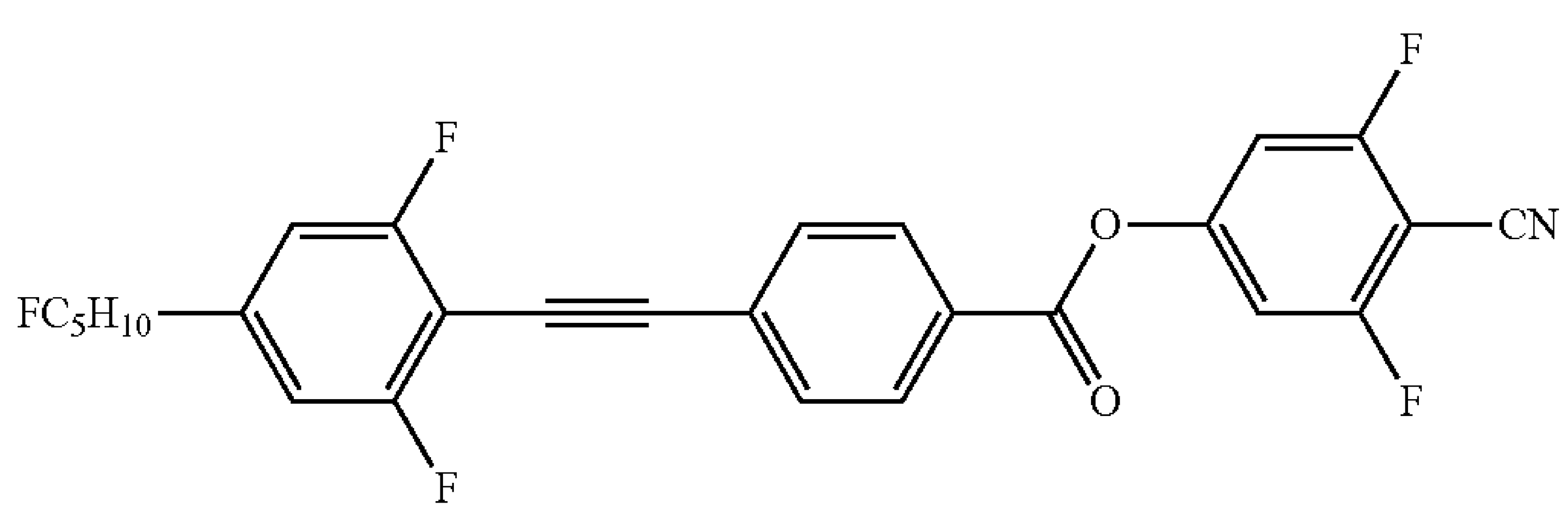

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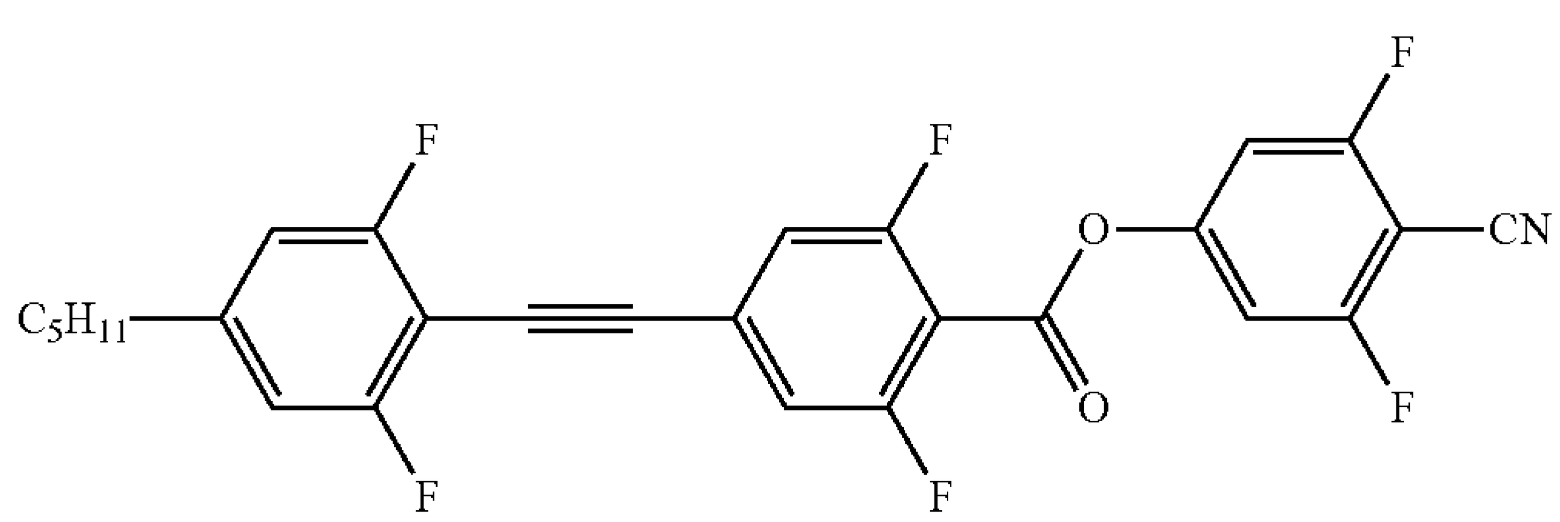

TABLE 1-continued

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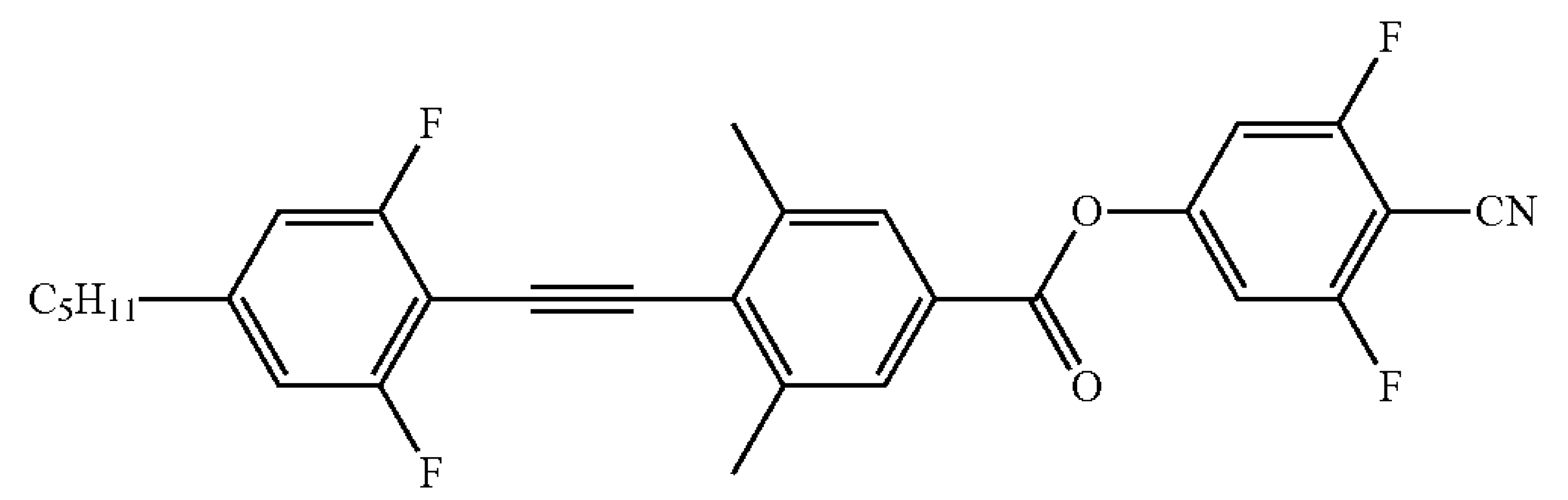

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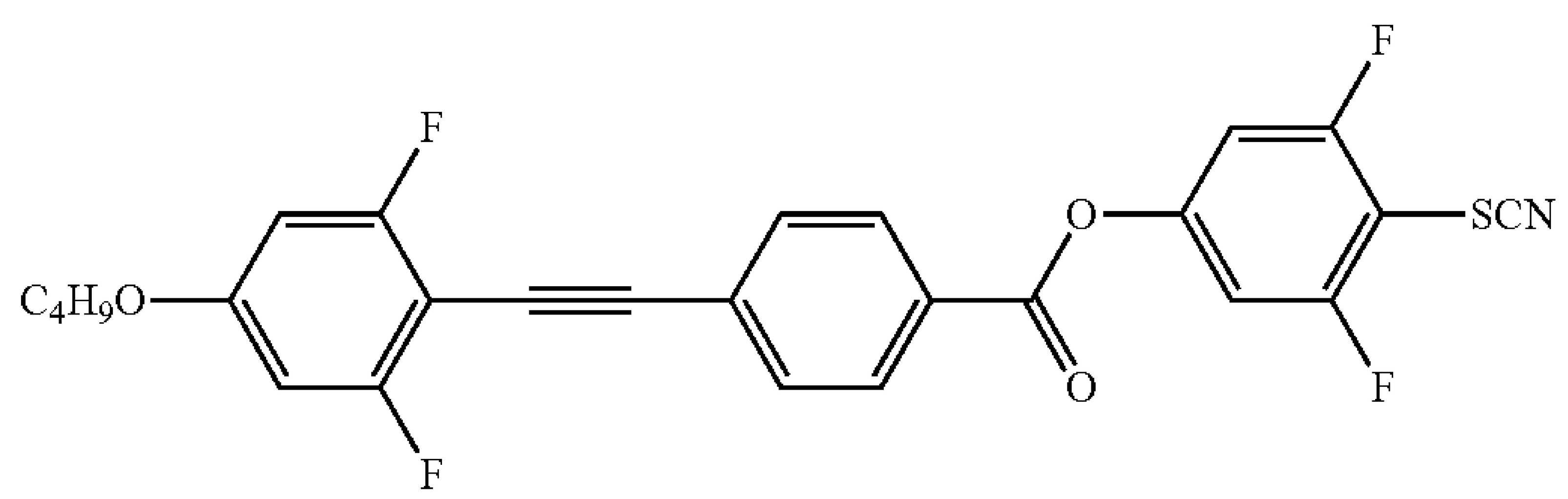

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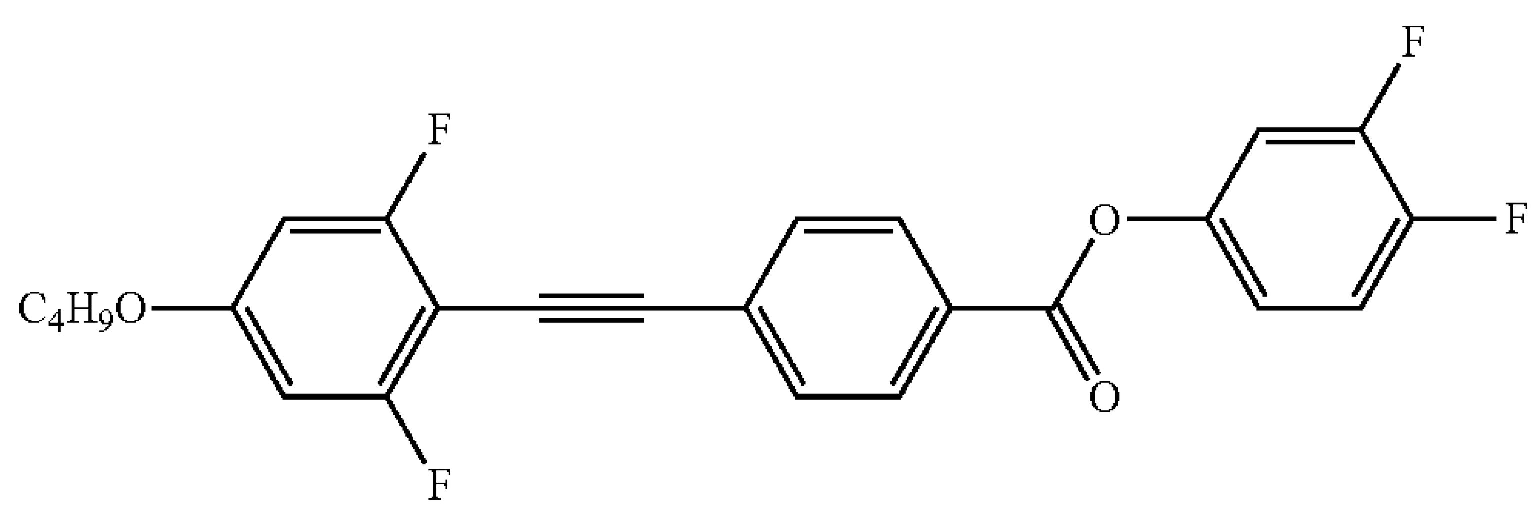

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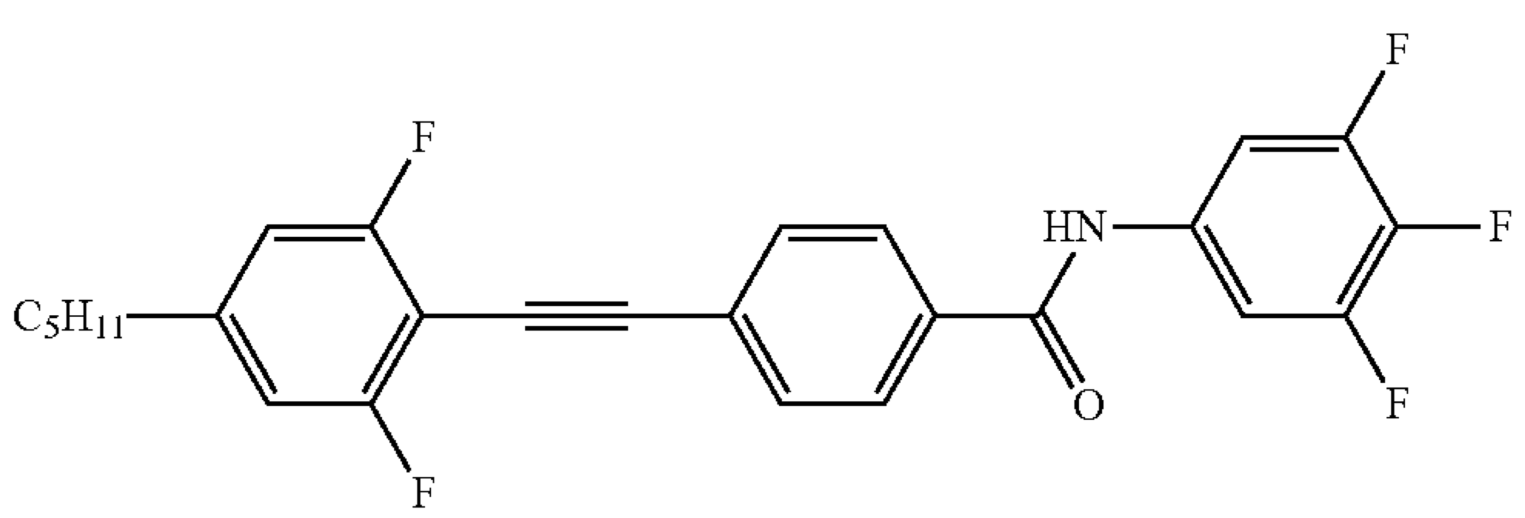

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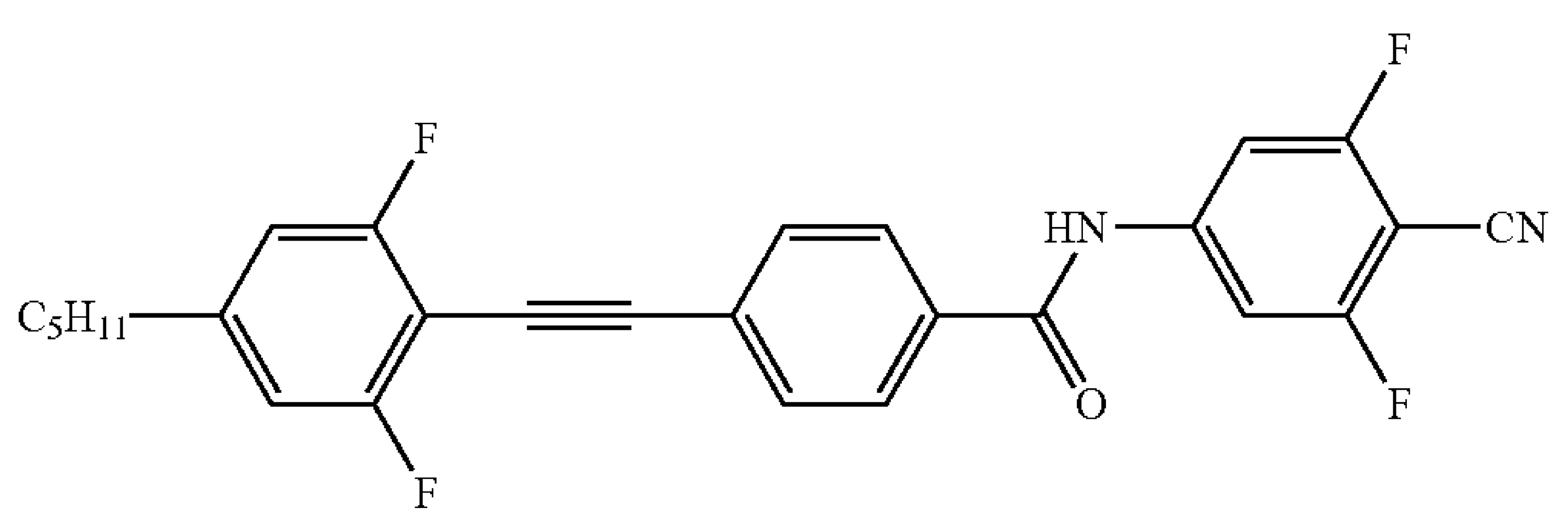
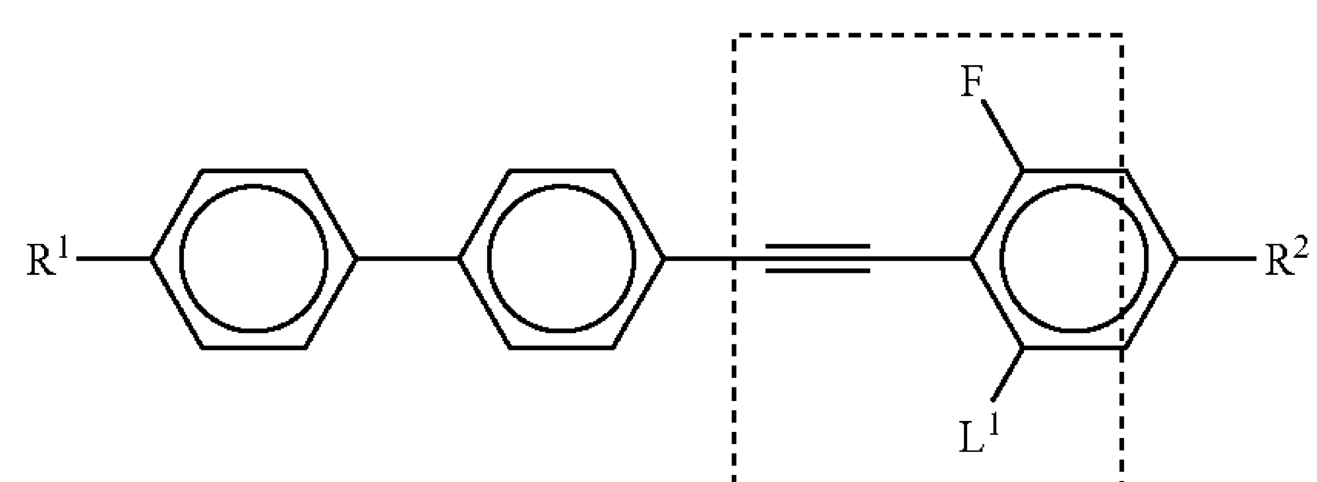


Experiments shows that the liquid crystal compounds according to various embodiments of the invention have unexpectedly high diamagnetic anisotropy compared to well-known liquid crystal compounds, and therefore they can be used to decrease a driving voltage of a liquid crystal display.

The following formula (II) presents a known liquid crystal compound (referred to Germany Patent Application No. 10241721A1), wherein R^1 and R^2 may be C_1-C_5 alkyl, and L_1 may be fluorine. As show in formula (II), the liquid crystal compound has a fluorine substituted benzyl group and an alkyne group (as circled by the dotted line below), and the diamagnetic anisotropy of the liquid crystal compound is merely between 30 and 40. That is, the liquid crystal compound having a structure of formula (II) has a low diamagnetic anisotropy.

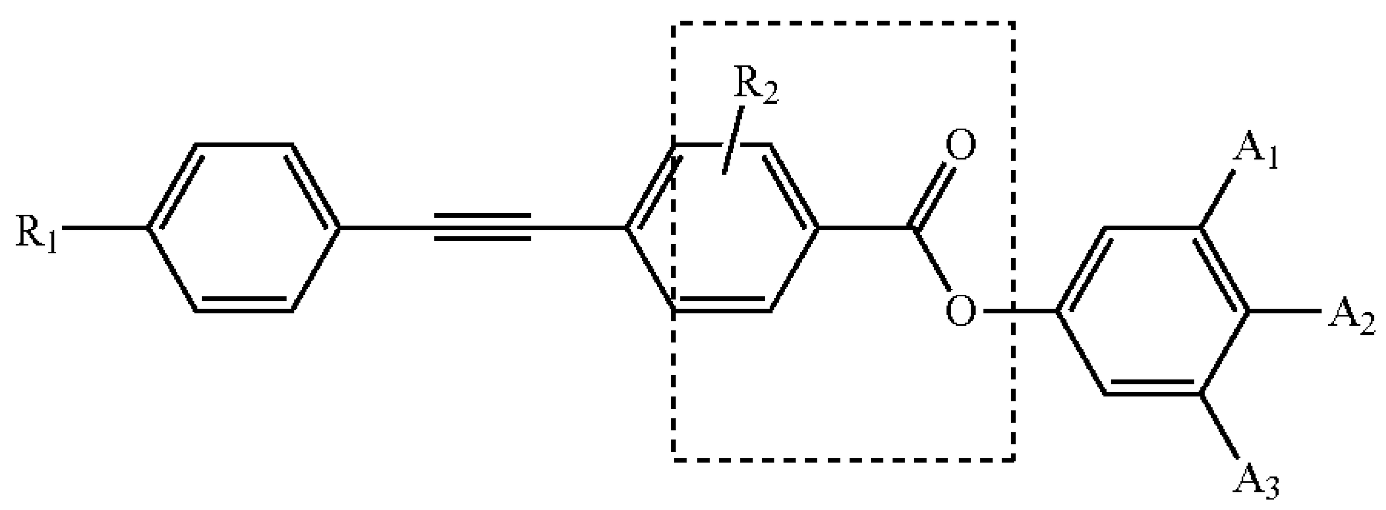
(II)



In addition, the following formula (III) presents another known liquid crystal compound (referred to Taiwan Patent Application TW I314577), wherein R^1 and R^2 may be C_1-C_{12} alkyl, and A_1, A_2, and A_3 may be halogen. As show in formula

(III), the liquid crystal compound has a benzyl group and —C(O)O— structure (as circled by the dotted line below), and the diamagnetic anisotropy of the liquid crystal compound is also merely between 30 and 40. That is, the liquid crystal compound having a structure of formula (III) also has a low diamagnetic anisotropy.

(III)



That is, according to the results of the known liquid crystal compounds (II) and (III), since both the liquid crystal compounds of formula (II) and formula (III) have low diamagnetic anisotropies, it was originally held assumed that a structure with a fluorine substituted benzyl group and an alkyne group as shown in formula (II) and a structure with a benzyl group and —C(O)O— structure as shown in formula (III) are structures that lead to low diamagnetic anisotropy.

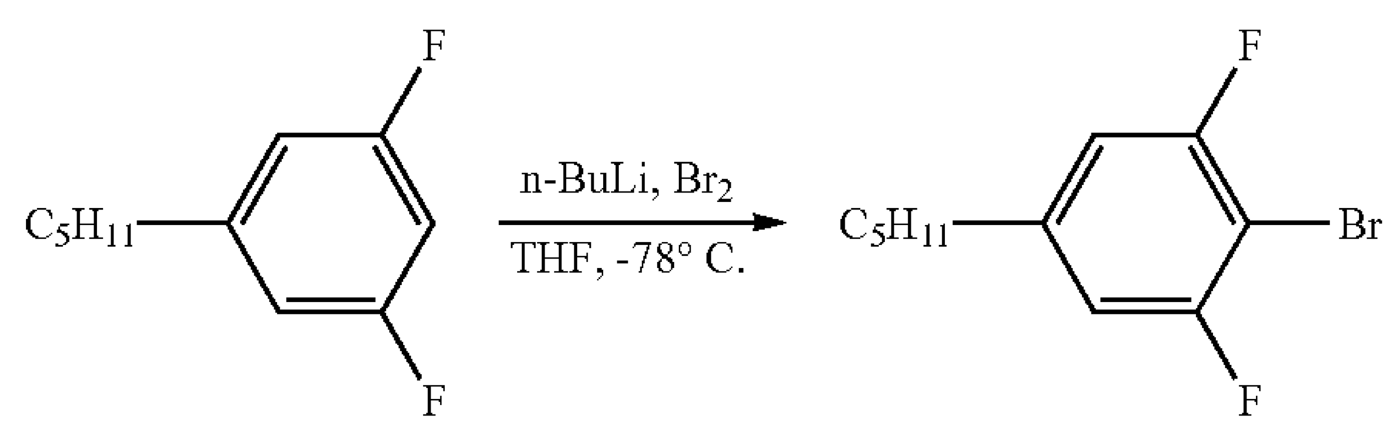
However, experiments surprisingly showed that the liquid crystal compounds having a structure of formula (I) including a fluorine substituted benzyl group, an alkyne group, and a —C(O)O— structure have unexpectedly high diamagnetic anisotropy, for example, above 45. Therefore, the liquid crystal compounds having a structure of formula (I) can be used in a liquid crystal display to decrease the driving voltage of the display.

FIG. **1** is a cross-section view of a liquid crystal display according to one embodiment of the invention. Referring to FIG. **1**, a liquid crystal display **100** includes a first substrate **102**, a second substrate **104**, and a liquid crystal layer **106**, wherein the second substrate **104** is disposed opposite to the first substrate **102**, and the liquid crystal layer **106** disposed between the first substrate **102** and the second substrate **104**. The liquid crystal layer **106** further includes a liquid crystal monomer and the liquid crystal compound having a structure of formula (I), wherein the liquid crystal monomer is different from the liquid crystal compound, and the liquid crystal layer contains 5% to 15% by weight of the liquid crystal compound. In one embodiment, the liquid crystal display is an active liquid crystal display including arrays of a plurality of pixels, wherein each pixel may include a thin film transistor and a storage capacitor. In another embodiment, the liquid crystal display is a passive liquid crystal display, wherein a first electrode is disposed on the first substrate along a first direction and a second electrode is disposed on the second substrate along a second direction, perpendicular to the first direction. However, these structures of the liquid crystal displays are, of course, merely examples and are not intended to be limiting. Any well-known or future developed liquid crystal display structure can be used. For example, the liquid crystal display structures described in United States Patent Publication No. 20080122998 or No. 20110058136 can also be used.

Example 1

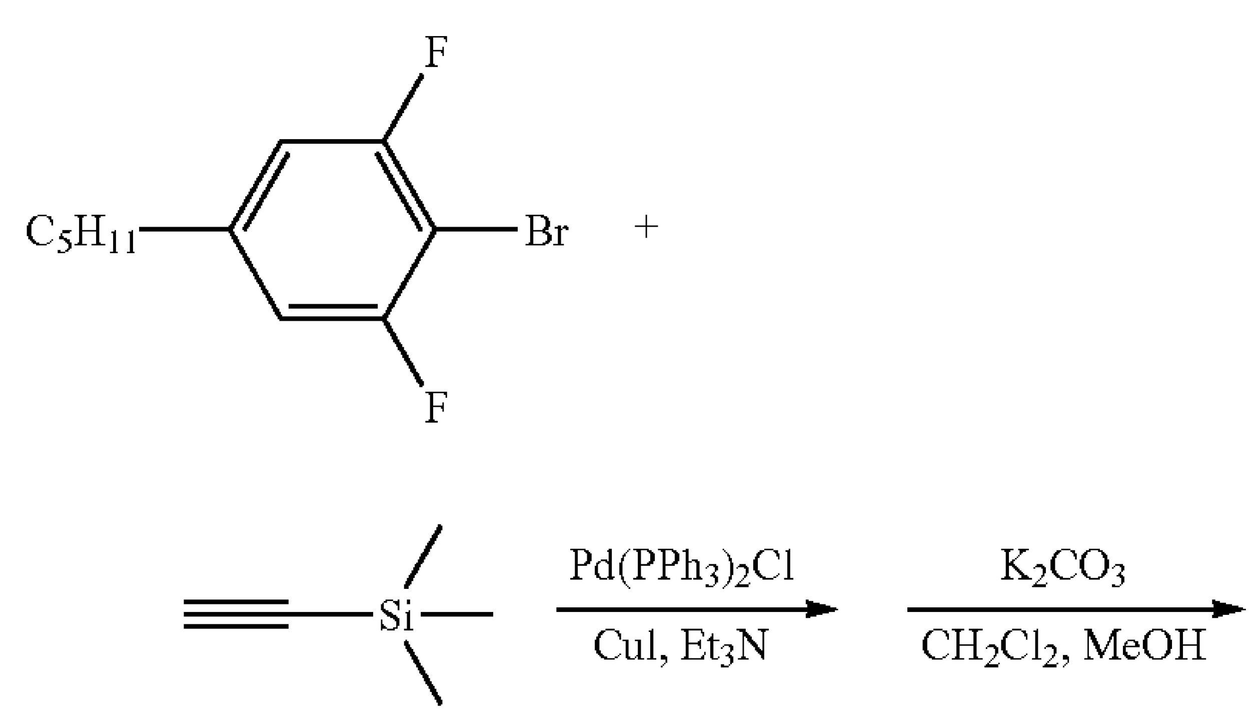
Synthesis of the Liquid Crystal Compound 1

1,3-difluoro-5-pentylbenzene (18.4 g; 100 mmol) and dried tetrahydrofuran (THF; 75 ml) were added into a reaction flask. After the 1,3-difluoro-5-pentylbenzene was dissolved, the solution was cooled to −78° C. When the temperature of the flask reached −78° C., n-butyllithium (66.4 ml; 110 mmol) was then added into the flask. The reaction continued under a low temperature for 1 hr, and the transparent liquid transferred into a white salt. Bromine (23.97 ml; 150 mmol) was then slowly added into the flask dropwise, and the reaction continued under a low temperature for 2 hrs. After 2 hrs, a temperature of the solution was raised back to room temperature, and the reaction was completed. After the reaction, ethyl acetate and water was used to extract the solution, and the resulting organic layer was concentrated under reduced pressure to obtain a brown liquid product. The reaction can be expressed by the following eqation:



Next, the resulting brown product (17.68 g; 80 mmol) and dried triethylamine (60 ml) was added into a reaction flask under N_2 atmosphere. Then, bis(triphenylphosphine)palladium dichloride ($Pd(PPh_3)_2Cl_2$; 0.55 g; 0.8 mmol; yellow solid) and copper iodide (0.15 g; 0.8 mmol; white solid) were added into the flask and stirred for 0.5 hrs. Then, ethynyltrimethylsilane (22.4 ml; 160 mmol) was added dropwise into the flask. The solution was then heated to 77° C. and the reaction continued for 6 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a brown product.

The resulting brown product (19.68 g; 75 mmol) was added into 100 ml of a solvent containing dichloromethane: methanol=1:1 and the resulting solution was stirred until the solid was dissolved. Then, K_2CO_3 (12.16 g; 88 mmol) was added into the solution and the resulting solution was stirred for 4 hrs. After the reaction, dichloromethane and water were used to extract the product, and a product of a yellow liquid in an organic layer was then obtained. The reaction can be expressed by the following equation:



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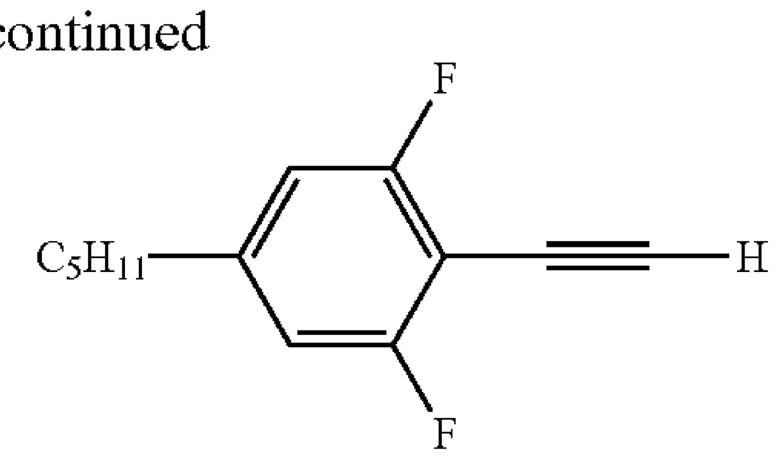
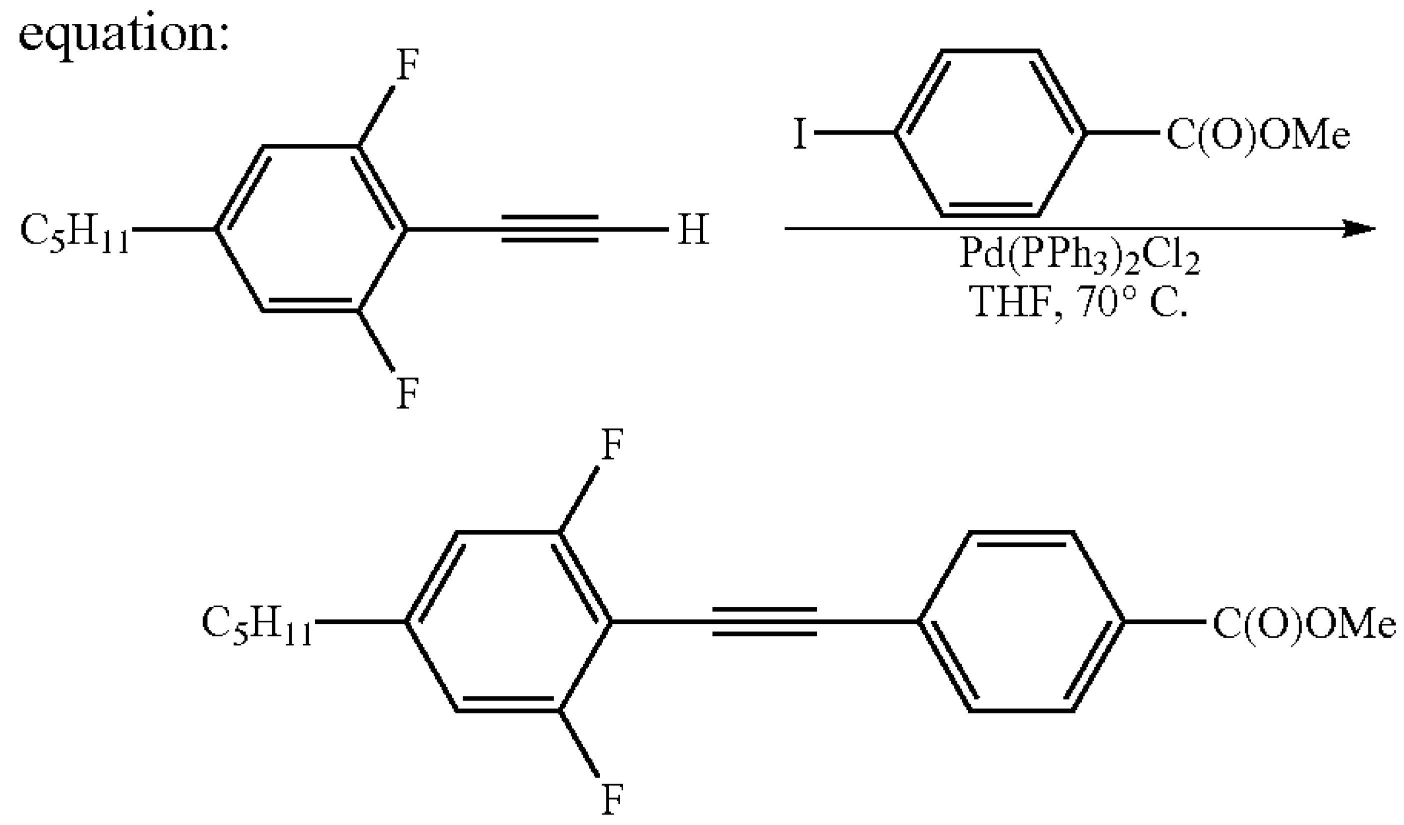
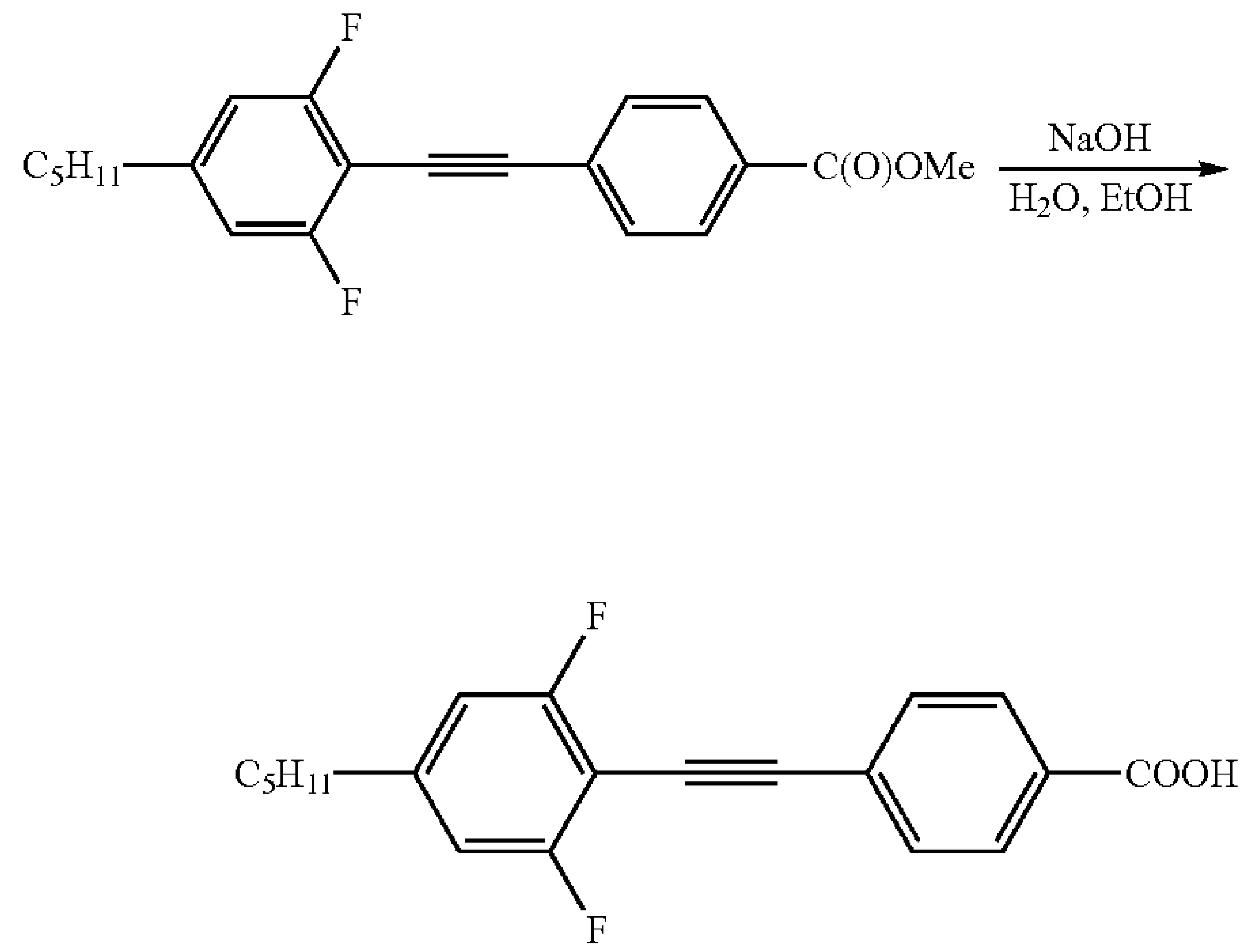


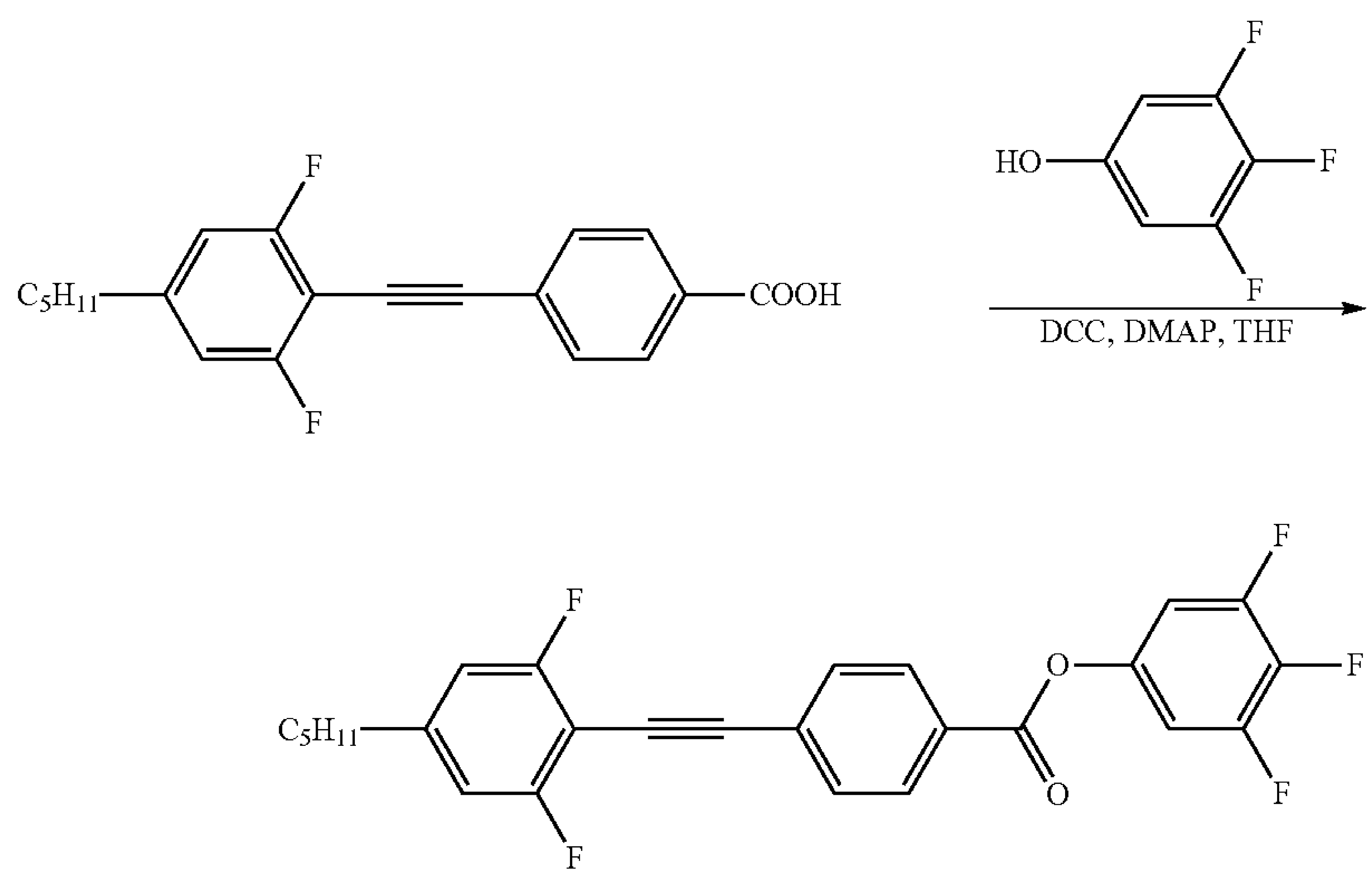
The resulting yellow liquid (17.12 g; 70 mmol), dried triethylamine (60 ml), and dried THF (60 ml) were added into a reaction flask under N_2 atmosphere. Bis(triphenylphosphine)palladium dichloride (0.51 g; 0.7 mmol) and copper iodide (0.14 g; 0.7 mmol) were then added into the flask, and the mixture was stirred for 0.5 hrs. Then, methyl 4-iodobenzoate (19.6 g; 75 mmol) was added into the solution and the resulting solution was heated to 70° C. The reaction continued for 12 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a yellow solid product. The reaction can be expressed by the following equation:



The resulting yellow product was then dissolved in a solution of water: ethanol=1:1 (60 ml), and NaOH (3.6 g; 150 mmol) was added into the solution. The solution was then heated to 60° C. The reaction was continued for 4 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a white solid product. The reaction can be expressed by the following equation:



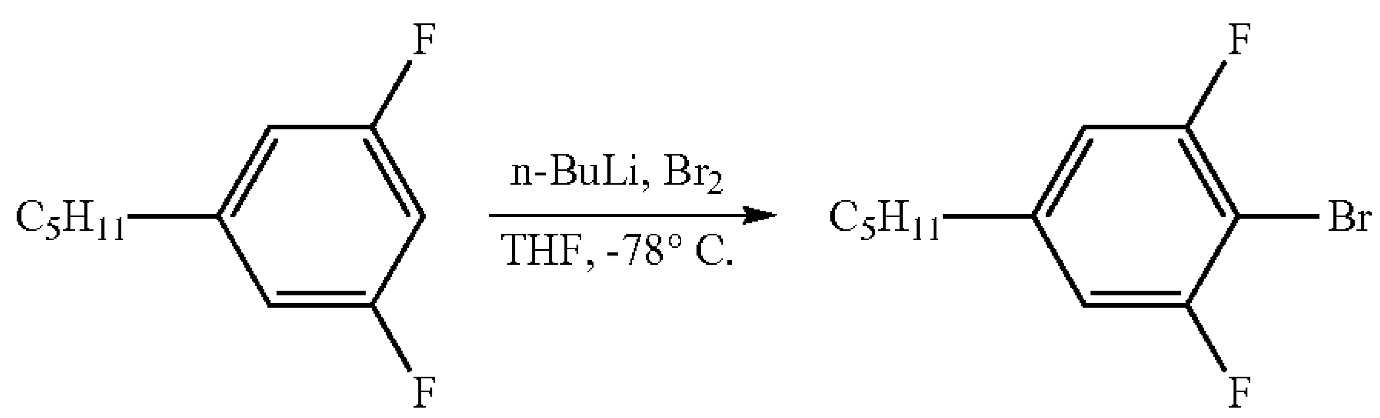
The resulting white product (19.7 g; 60 mmol) and dried THF (50 ml) were added into a reaction flask under N_2 atmosphere. Then, 3, 4, 5,-trifluorophenol, as a white solid, (8.8 g; 60 mmol), 4-(dimethylamino)pyridine (DMPA; 2.9 g; 24 mmol), and dicyclohexylcarbodiimide (DCC; 14.8 g; 72 mmol) were added into the solution. The solution was then heated to 70° C. The reaction was continued for 6 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure. A yellow solid product was then obtained as a crude product. The crude product was recrystallized twice by hexane and dichloromethane to obtain a liquid crystal compound 1 as a white solid (19.7 g; 43 mmol; yield: 43%). The reaction can be expressed by the following equation:



Example 2

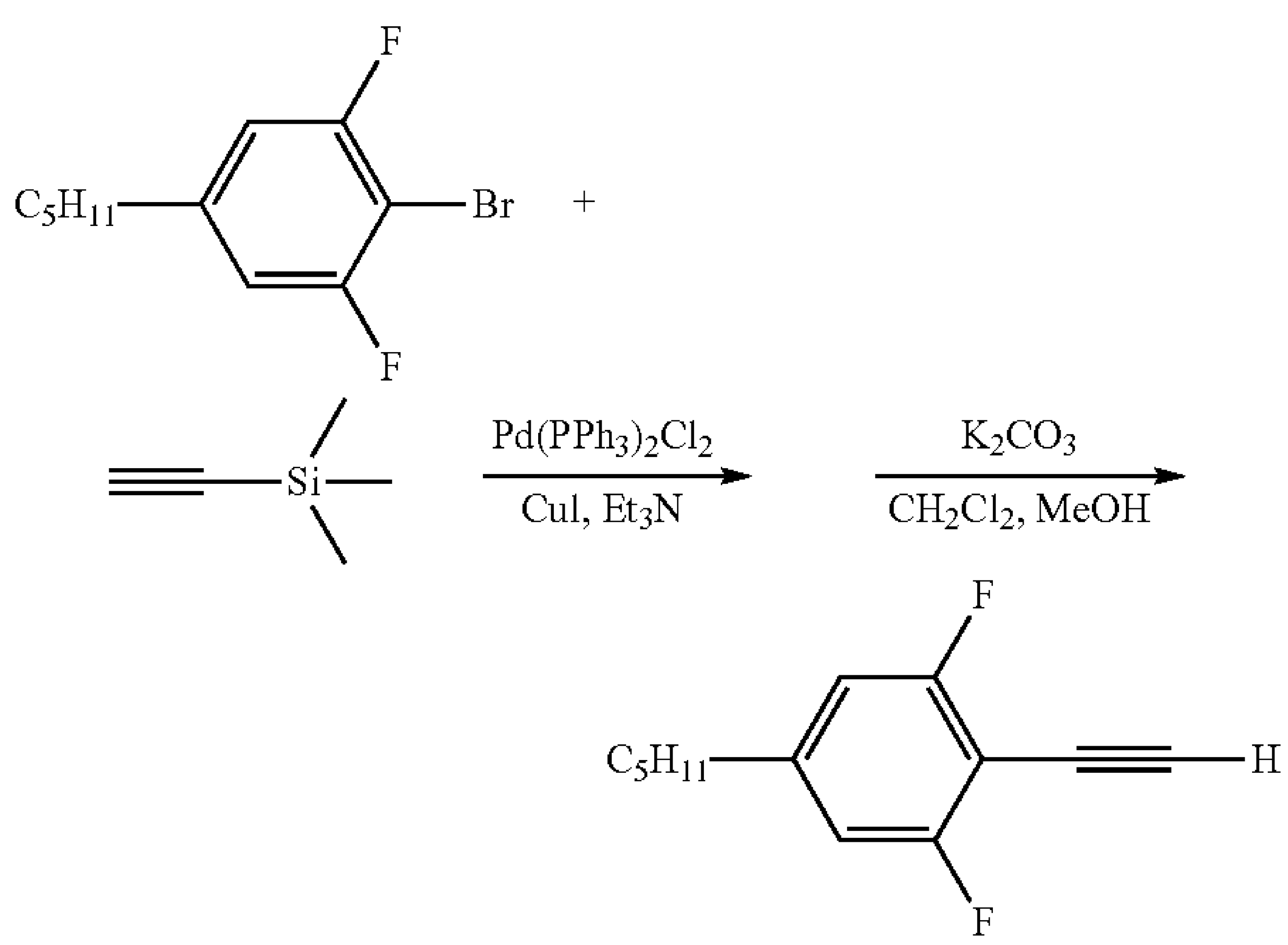
Synthesis of the Liquid Crystal Compound 2

1,3-difluoro-5-pentylbenzene (18.4 g; 100 mmol) and dried tetrahydrofuran (THF; 75 ml) were added into a reaction flask. After the 1,3-difluoro-5-pentylbenzene was dissolved, the solution was cooled to −78° C. When the temperature of the solution reached −78° C., n-butyllithium (66.4 ml; 110 mmol) was then added into the flask. The reaction continued under a low temperature for 1 hr, and the transparent liquid transferred into a white salt. Bromine (23.97 ml; 150 mmol) was then slowly added into the flask dropwise, and the reaction continued under a low temperature for 2 hrs. After 2 hrs, a temperature of the solution was put back to room temperature, and the reaction was completed. After the reaction, ethyl acetate and water was used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a brown liquid product. The reaction can be expressed by the following equation:

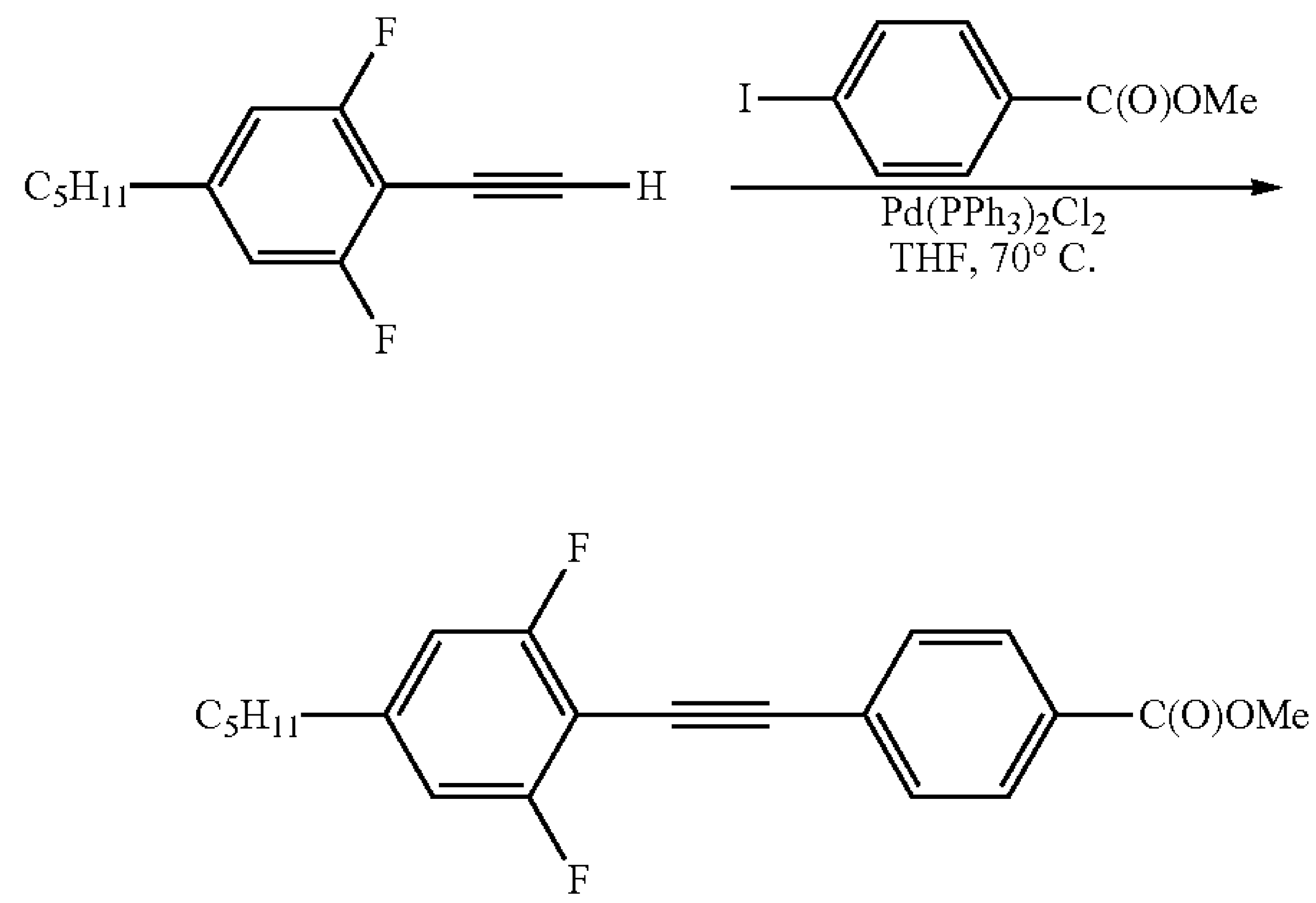


Next, the resulting brown product (17.68 g; 80 mmol) and dried triethylamine (60 ml) was added into a reaction flask under N_2 atmosphere. Then, bis(triphenylphosphine)palladium dichloride ($Pd(PPh_3)_2Cl_2$; 0.55 g; 0.8 mmol) and copper iodide (0.15 g; 0.8 mmol) were added into the flask and stirred for 0.5 hrs. Then, ethynyltrimethylsilane (22.4 ml; 160 mmol) was added dropwise into the flask. The solution was then heated to 77° C. and the reaction continued for 6 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a brown product.

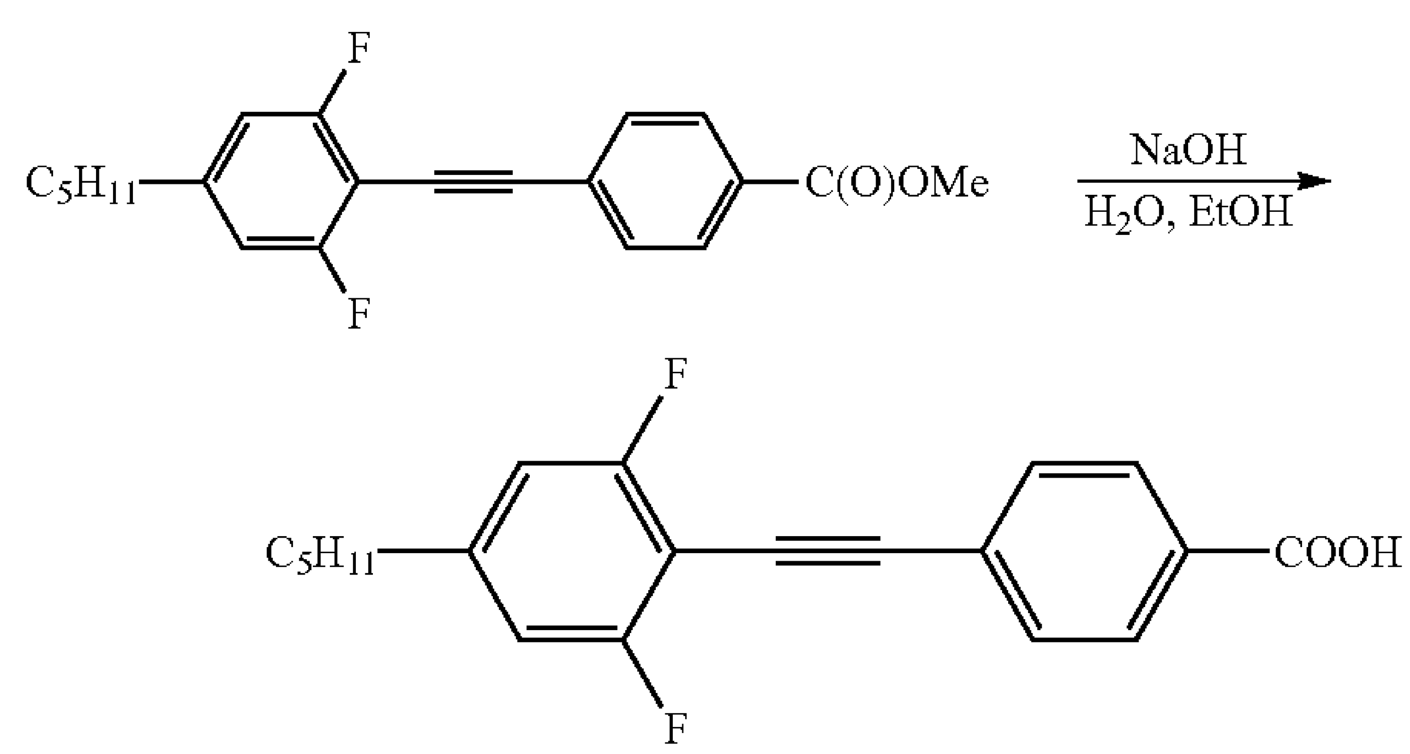
The resulting brown product (19.68 g; 75 mmol) was added into 100 ml of a solvent containing dichloromethane: methanol=1:1 and the resulting solution was stirred until the solid was dissolved. Then, K_2CO_3 (12.16 g; 88 mmol) was added into the solution and the resulting solution was stirred for 4 hrs. After the reaction, dichloromethane and water were used to extract the product, and a product of a yellow liquid was then obtained in the organic layer. The reaction can be expressed by the following equation:



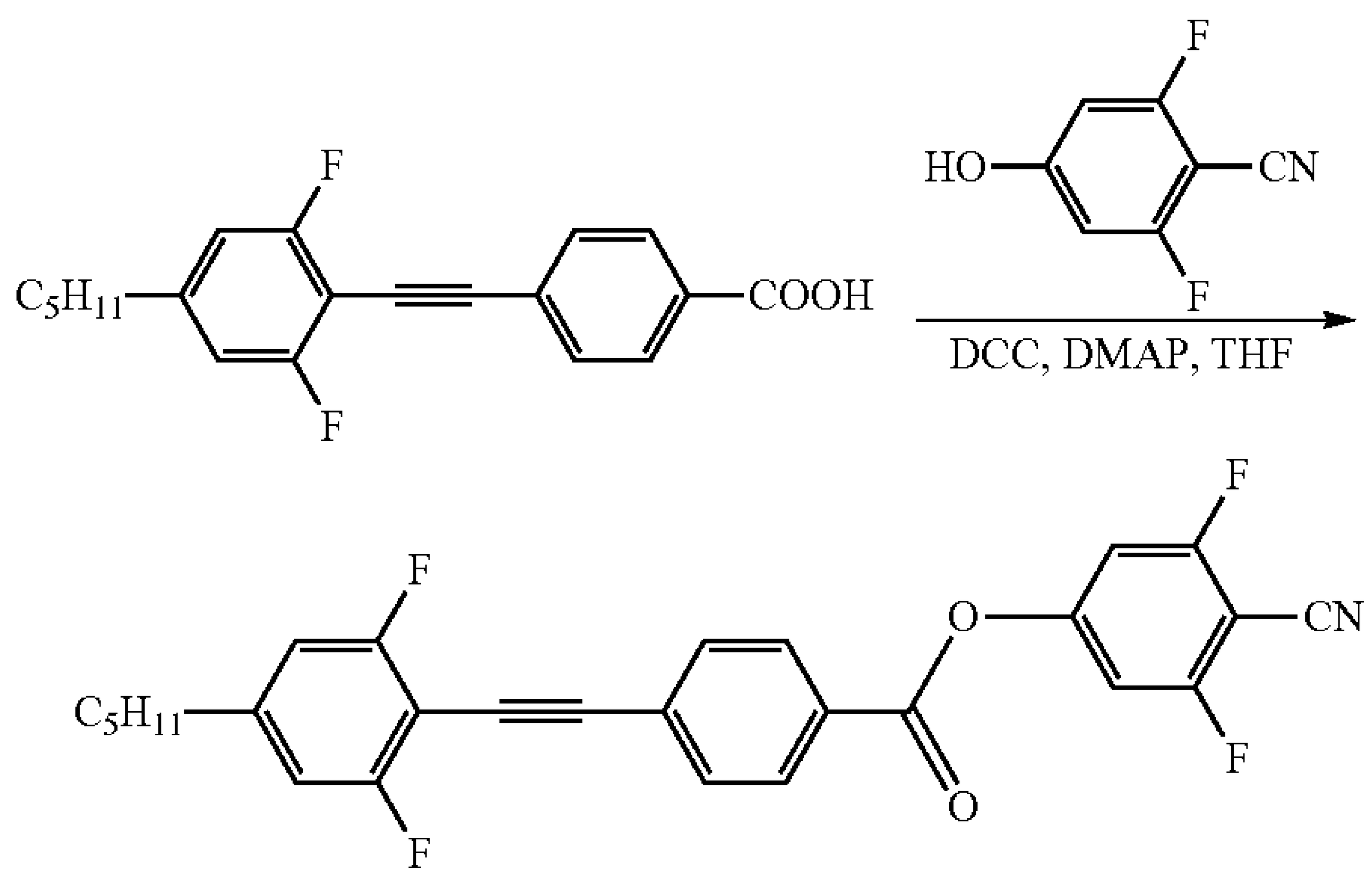
The resulting yellow liquid (17.12 g; 70 mmol), dried triethylamine (60 ml), and dried THF (60 ml) were added into a reaction flask under N_2 atmosphere. Bis(triphenylphosphine)palladium dichloride (0.51 g; 0.7 mmol) and copper iodide (white solid; 0.14 g; 0.7 mmol) were then added into the flask, and the mixture was stirred for 0.5 hrs. Then, methyl 4-iodobenzoate (19.6 g; 75 mmol) was added into the solution and the resulting solution was heated to 70° C. The reaction was continued for 12 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a yellow solid product. The reaction can be expressed by the following equation:



The resulting yellow product was then dissolved in a solution of water ethanol=1:1 (60 ml), and NaOH (3.6 g; 150 mmol) was added into the solution. The solution was then heated to 60° C. The reaction was continued for 4 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a white solid product. The reaction can be expressed by the following equation:



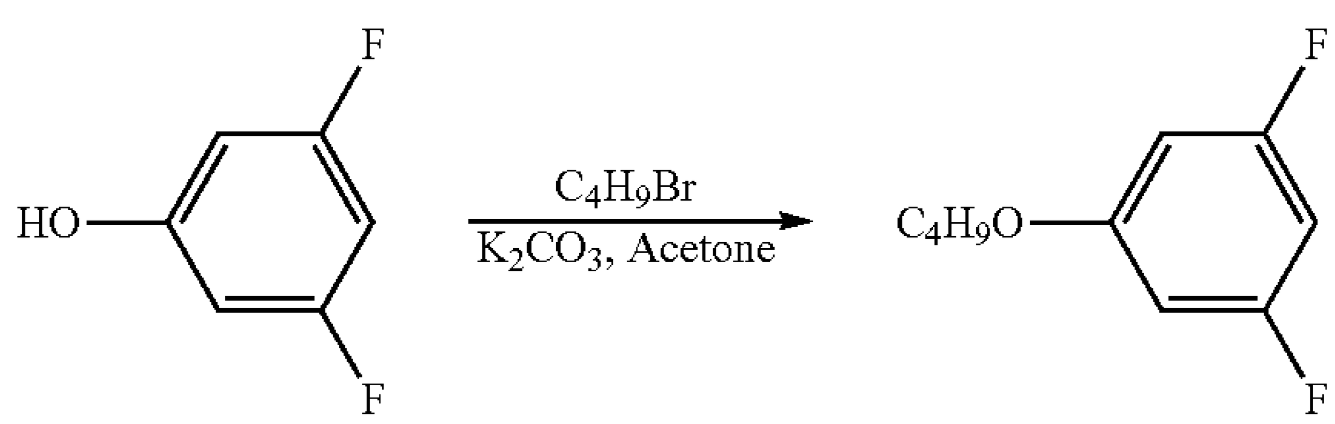
The resulting white product (19.7 g; 60 mmol) and dried THF (50 ml) were added into a flask. After the white product was dissolved, 4-cyano-3,5-difluorophenol (9.3 g; 60 mmol), 4-(dimethylamino)pyridine (DMPA; 2.9 g; 24 mmol), and dicyclohexylcarbodiimide (DCC; 14.8 g; 72 mmol) were added into the solution under N_2 atmosphere. The solution was then heated to 70° C. The reaction was continued for 6 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure. A yellow solid product was then obtained as a crude product. The crude product was recrystallized twice by hexane and dichloromethane to obtain the liquid crystal compound 2 as a white solid (20.9 g; 45 mmol; yield: 45%). The reaction can be expressed by the following equation:



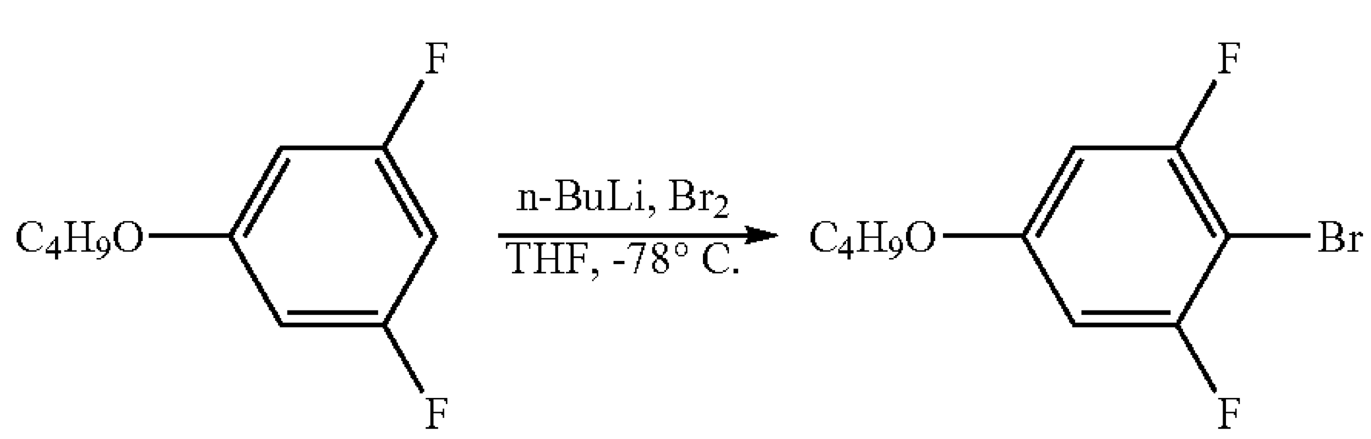
Example 3

Synthesis of the Liquid Crystal Compound 3

3,5-difluorophenol (14.3 g; 110 mmol), K_2CO_3 (22.80 g; 165 mmol), and acetone (100 ml) were added into a reaction flask. 1-bromobutane (15.1 ml; 110 mmol) was added into the flask dropwise. The solution was heated to 60° C. and the reaction continued for 6 hrs. After the reaction, ethyl acetate and water was used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a white liquid product. The reaction can be expressed by the following equation:

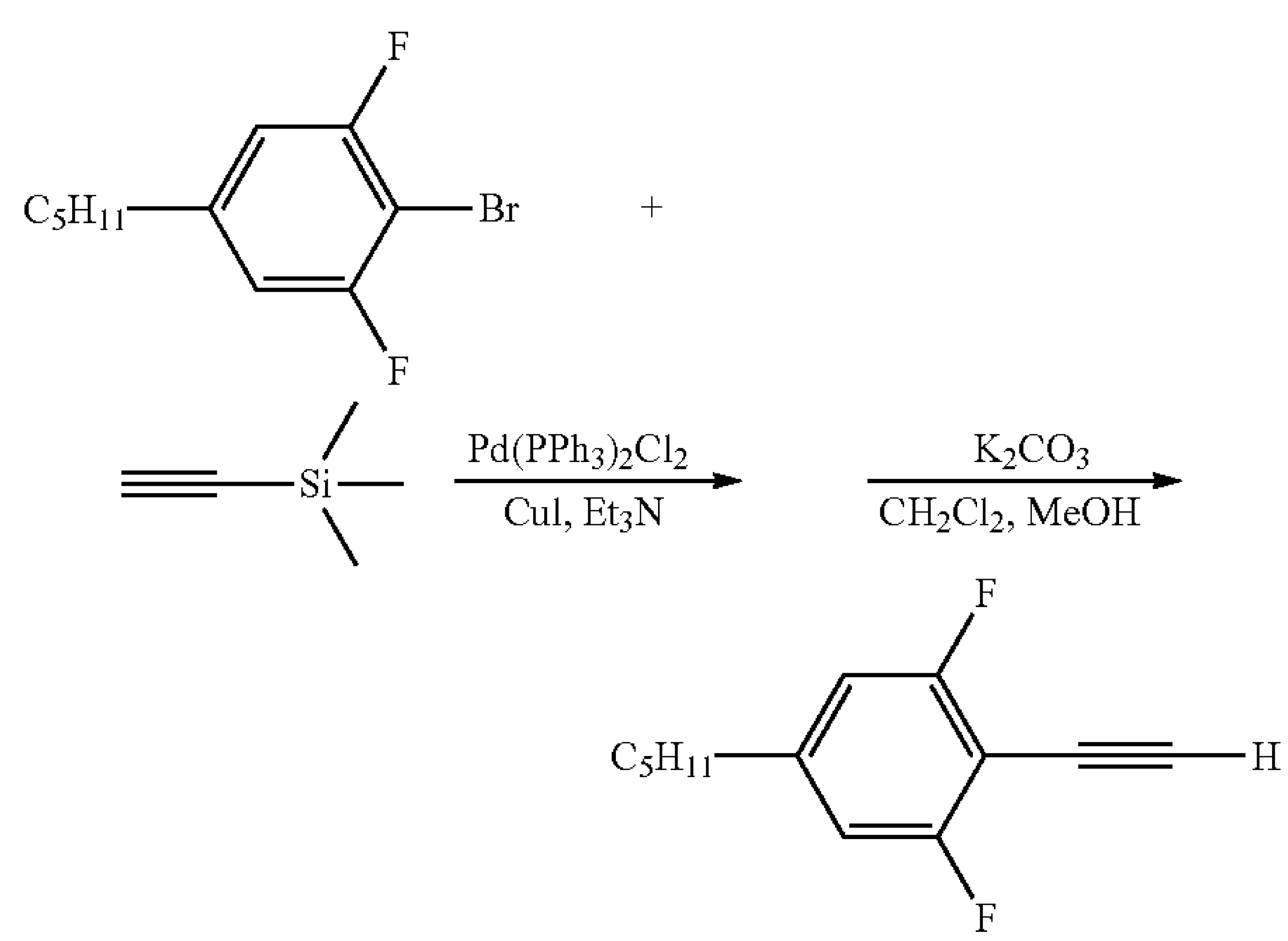


The resulting white liquid (18.4 g; 100 mmol) and dried tetrahydrofuran (THF; 75 ml) were added into a reaction flask. Then, the solution was cooled to −78° C. When the temperature of the solution reached −78° C., n-butyllithium (66.4 ml; 110 mmol) was then added into the flask. The reaction continued under a low temperature for 1 hr, and the transparent liquid transferred into a white salt. Bromine (23.97 ml; 150 mmol) was then slowly added into the flask dropwise, and the reaction continued under a low temperature for 2 hrs. After 2 hrs, a temperature of the solution was raised back to room temperature, and the reaction was completed. After the reaction, ethyl acetate and water was used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a brown liquid product. The reaction can be expressed by the following equation:

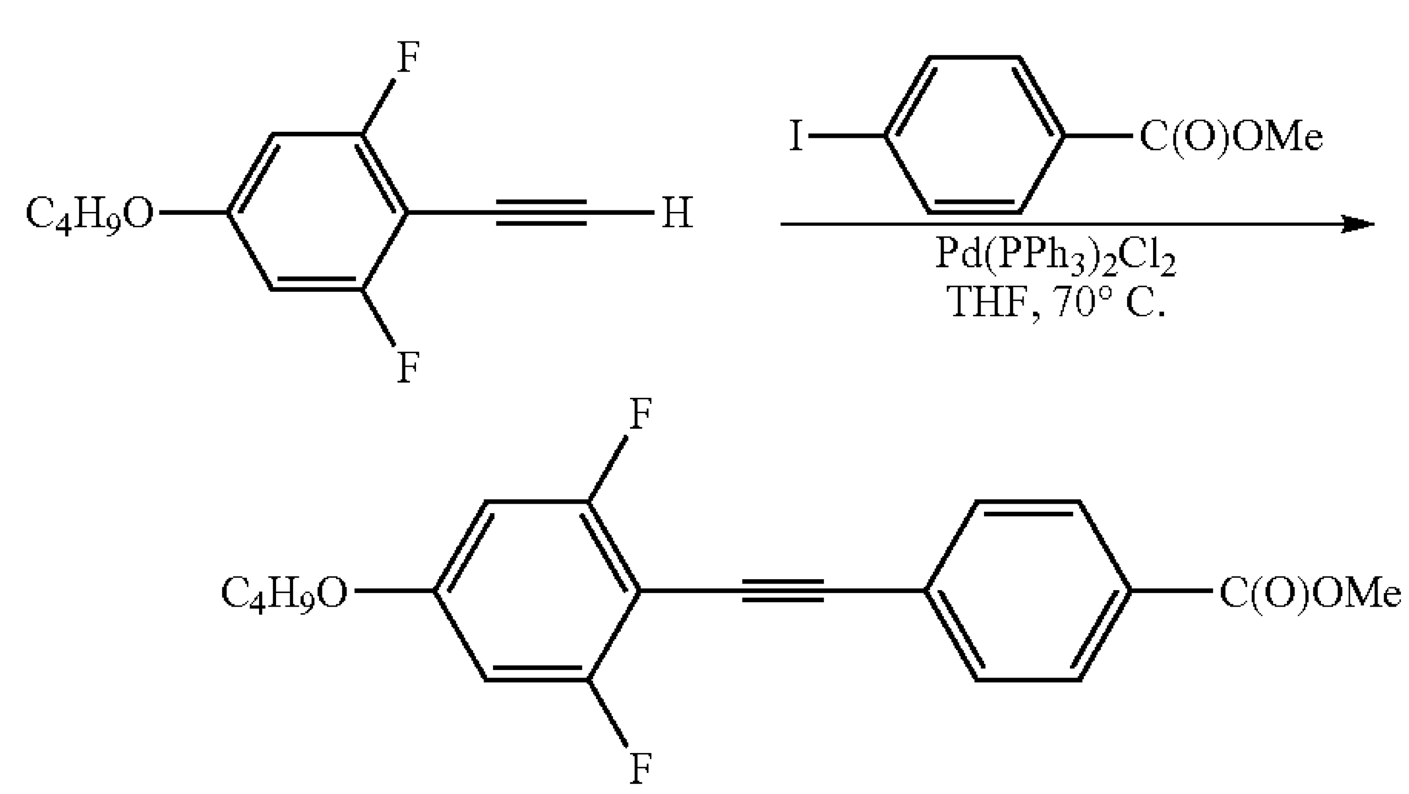


Next, the resulting brown product (17.68 g; 80 mmol) and dried triethylamine (60 ml) was added into a reaction flask under N_2 atmosphere. Then, bis(triphenylphosphine)palladium dichloride (0.55 g; 0.8 mmol) and copper iodide (0.15 g; 0.8 mmol) were added into the flask and stirred for 0.5 hrs. Then, ethynyltrimethylsilane (22.4 ml; 160 mmol) was added dropwise into the flask. The solution was then heated to 77° C. and the reaction continued for 6 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a brown product.

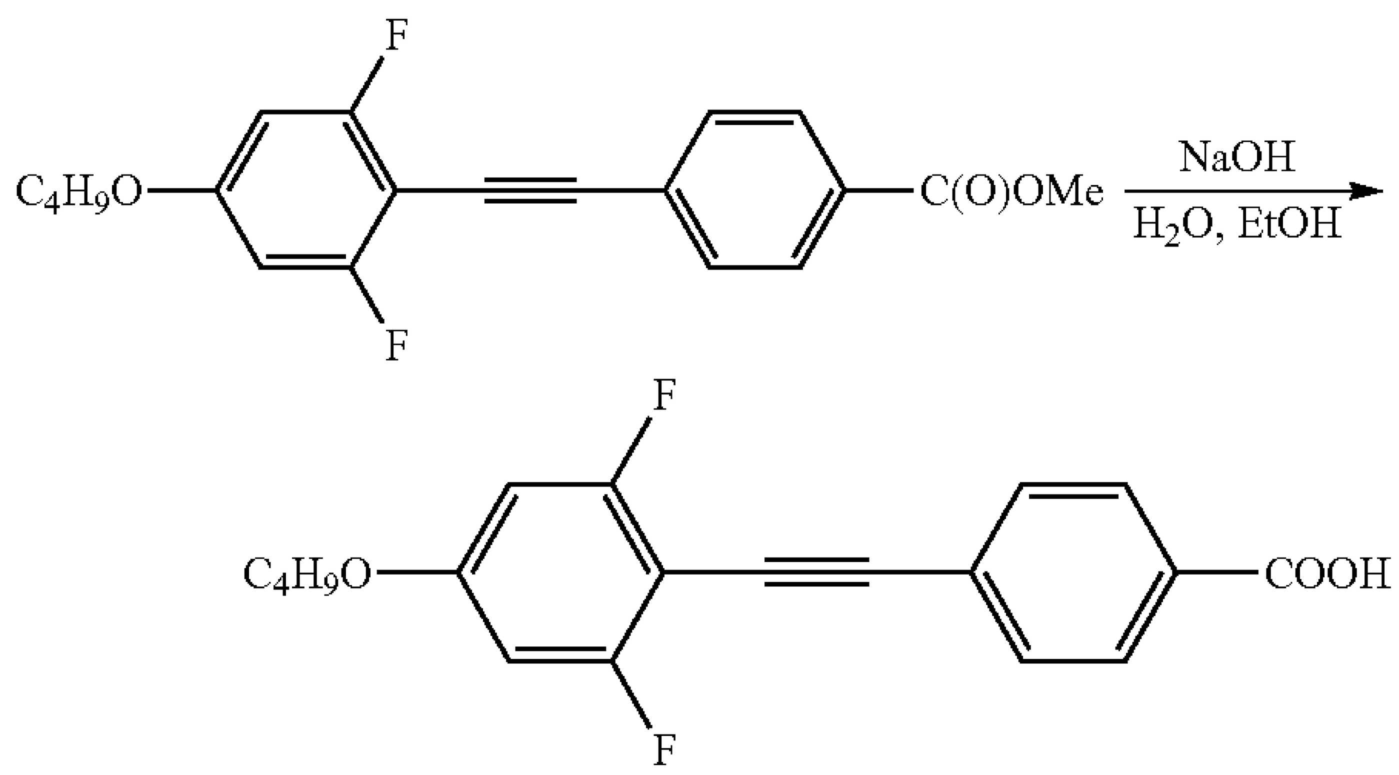
The resulting brown product (19.68 g; 75 mmol) was added into 100 ml of a solvent containing dichloromethane: methanol=1:1 and the resulting solution was stirred until the solid was dissolved. Then, K_2CO_3 (12.16 g; 88 mmol) was added into the solution and the resulting solution was stirred for 4 hrs. After the reaction, dichloromethane and water were used to extract the product, and a product of a yellow liquid in an organic layer was then obtained. The reaction can be expressed by the following equation:



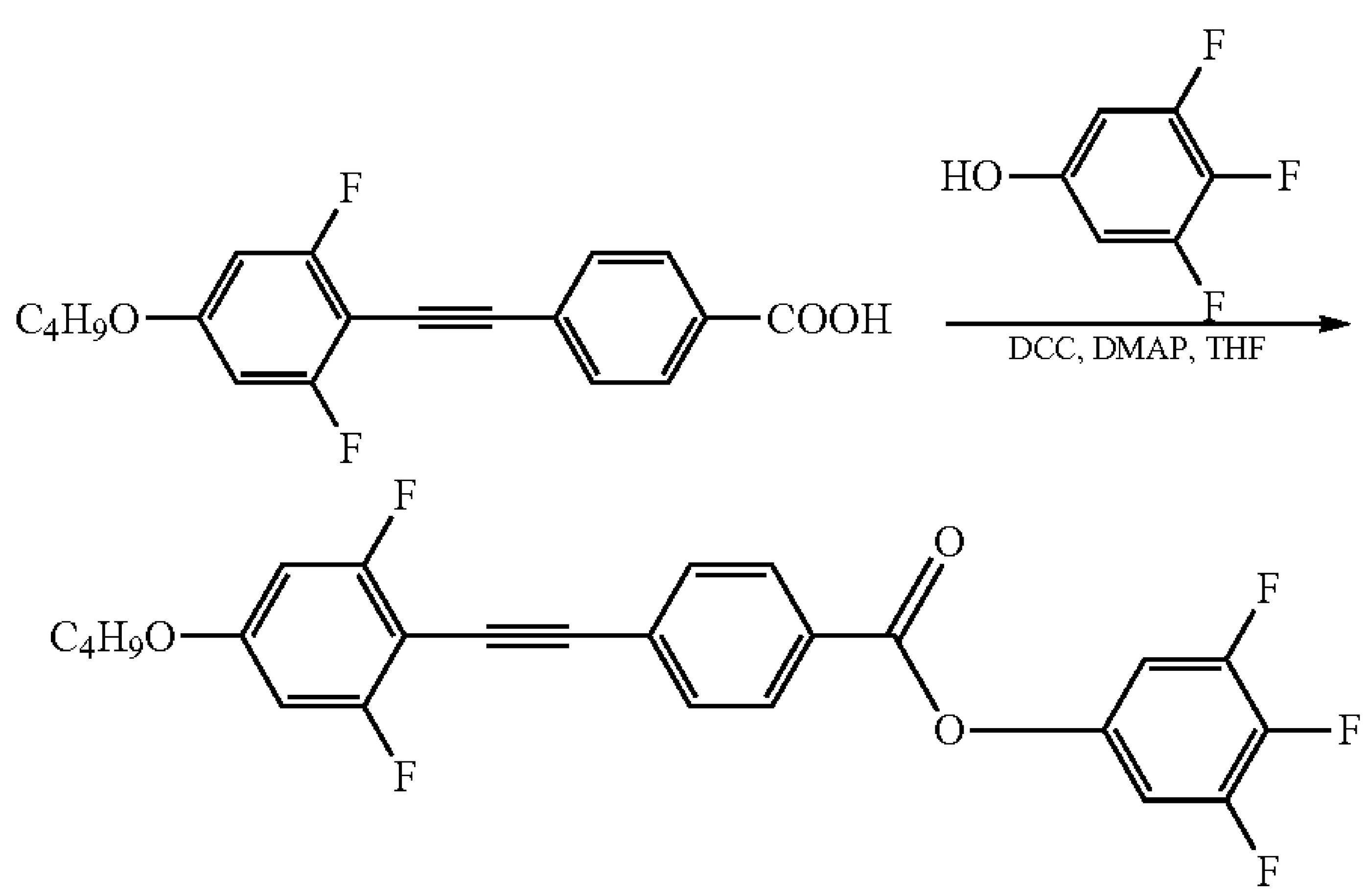
The resulting yellow liquid (17.12 g; 70 mmol), dried triethylamine (60 ml), and dried THF (60 ml) were added into a reaction flask under N_2 atmosphere. Bis(triphenylphosphine)palladium dichloride (0.51 g; 0.7 mmol) and copper iodide (white solid; 0.14 g; 0.7 mmol) were then added into the flask, and the mixture was stirred for 0.5 hrs. Then, methyl 4-iodobenzoate (19.6 g; 75 mmol) was added into the flask and the resulting solution was heated to 70° C. The reaction continued for 12 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a yellow solid product. The reaction can be expressed by the following equation:



The resulting yellow product was then dissolved in a solution of water: ethanol=1:1 (60 ml), and NaOH (3.6 g; 150 mmol) was added into the solution. The solution was then heated to 60° C. The reaction was continued for 4 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a white solid product. The reaction can be expressed by the following equation:



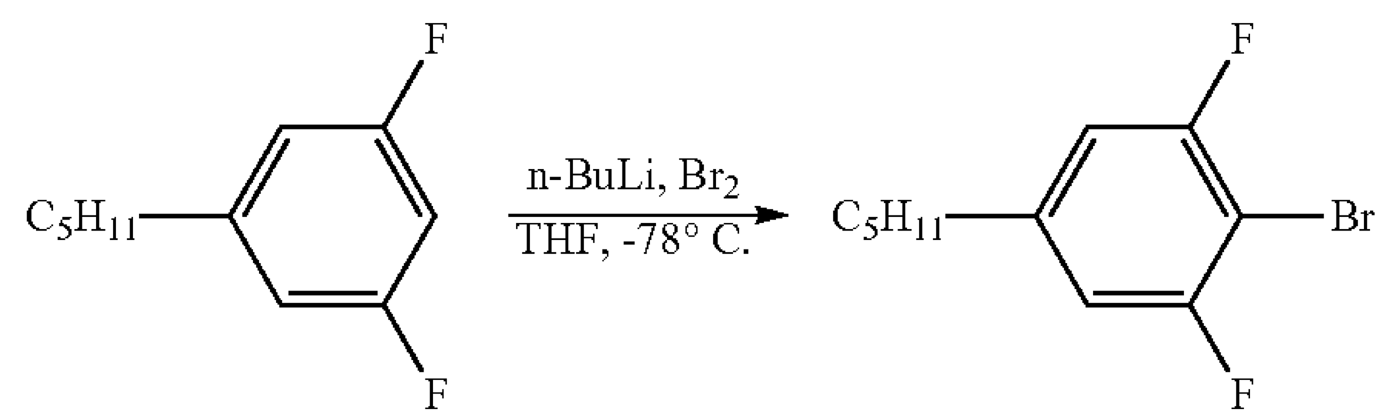
The resulting white product (19.7 g; 60 mmol) and dried THF (54-cyano-3,5-difluorophenol 3,4,5,-trifluorophenol (9.3 g; 60 mmol), 4-(dimethylamino)pyridine (DMPA; 2.9 g; 24 mmol), and dicyclohexylcarbodiimide (DCC; 14.8 g; 72 mmol) were added into the solution. The solution was then heated to 70° C. The reaction was continued for 6 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure. A yellow solid product was then obtained as a crude product. The crude product was recrystallized twice by hexane and dichloromethane to obtain a liquid crystal compound 3 as a light yellow solid (22.9 g; 49 mmol; yield: 44%). The reaction can be expressed by the following equation:



Example 4

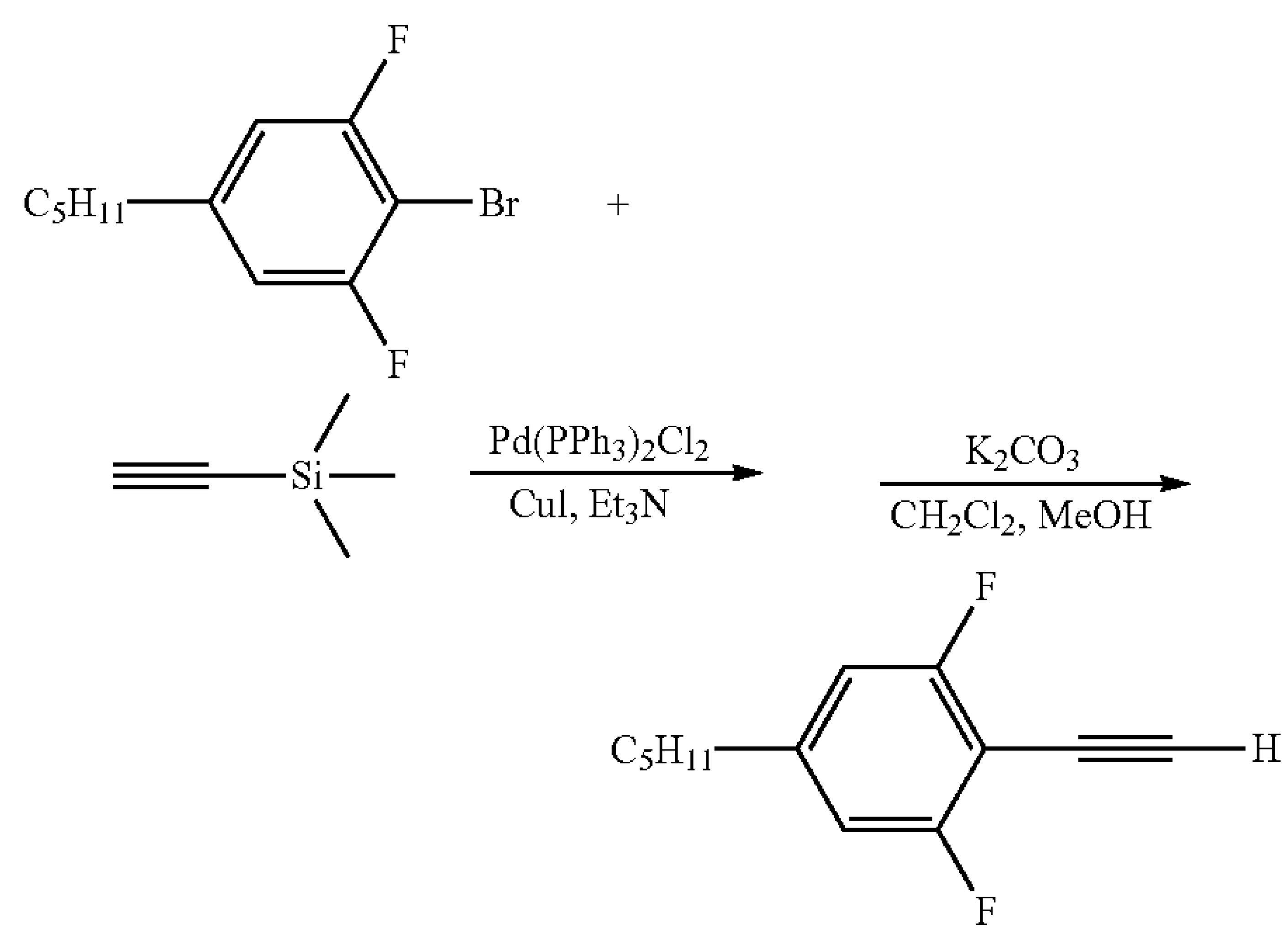
Synthesis of the Liquid Crystal Compound 17

1,3-difluoro-5-pentylbenzene (18.4 g; 100 mmol) and dried tetrahydrofuran (THF; 75 ml) were added into a reaction flask. After the 1,3-difluoro-5-pentylbenzene was dissolved, the solution was cooled to −78° C. When the temperature of the solution reached −78° C., n-butyllithium (66.4 ml; 110 mmol) was then added into the flask. The reaction continued under a low temperature for 1 hr, and the transparent liquid transferred into a white salt. Bromine (23.97 ml; 150 mmol) was then slowly added into the flask dropwise, and the reaction continued under a low temperature for 2 hrs. After 2 hrs, a temperature of the solution was put back to room temperature, and the reaction was completed. After the reaction, ethyl acetate and water was used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a brown liquid product. The reaction can be expressed by the following equation:

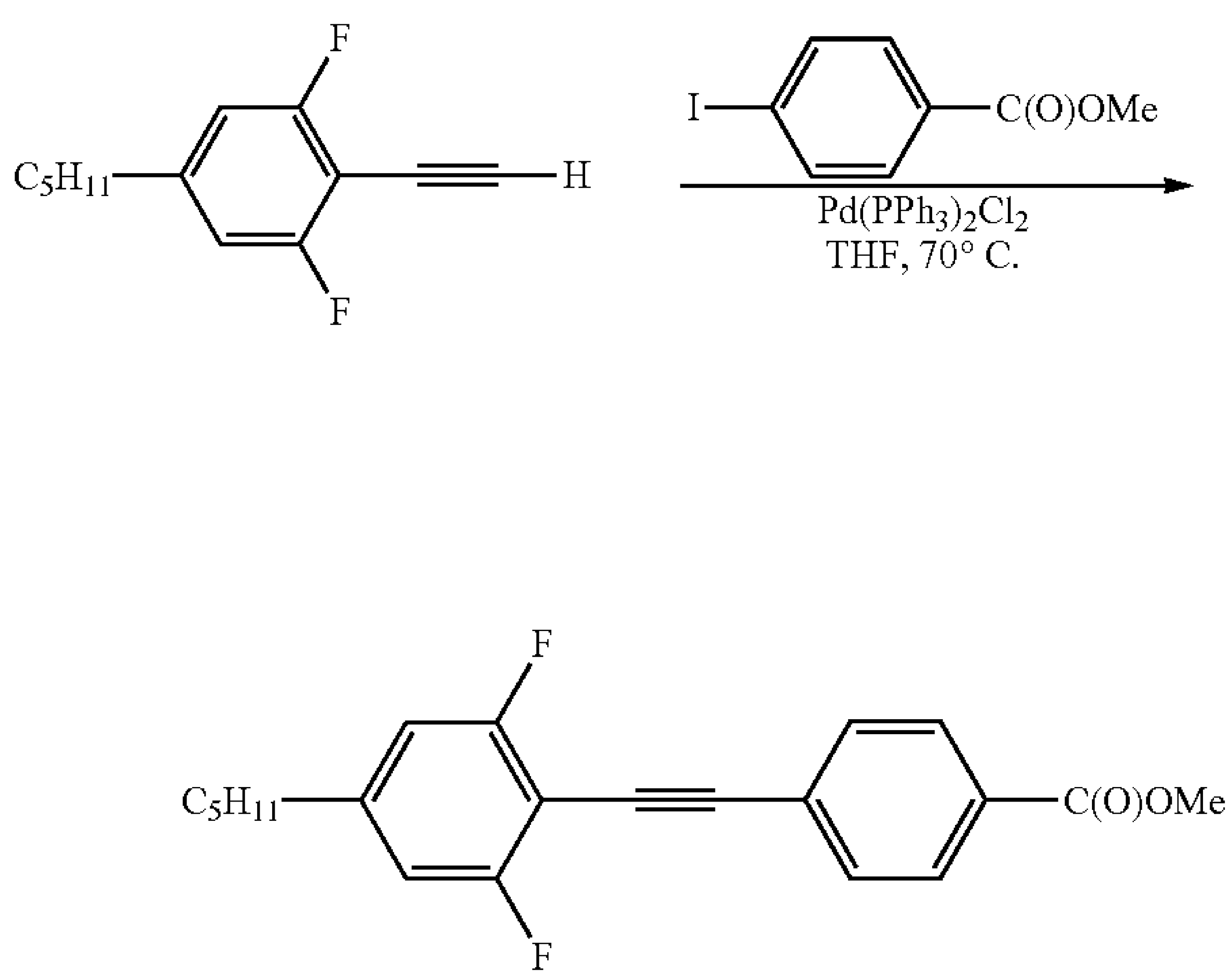


Next, the resulting brown product (17.68 g; 80 mmol) and dried triethylamine (60 ml) was added into a reaction flask under N_2 atmosphere. Then, bis(triphenylphosphine)palladium dichloride ($Pd(PPh_3)_2Cl_2$; 0.55 g; 0.8 mmol) and copper iodide (0.15 g; 0.8 mmol) were added into the flask and stirred for 0.5 hrs. Then, ethynyltrimethylsilane (22.4 ml; 160 mmol) was added dropwise into the flask. The solution was then heated to 77° C. and the reaction continued for 6 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a brown product.

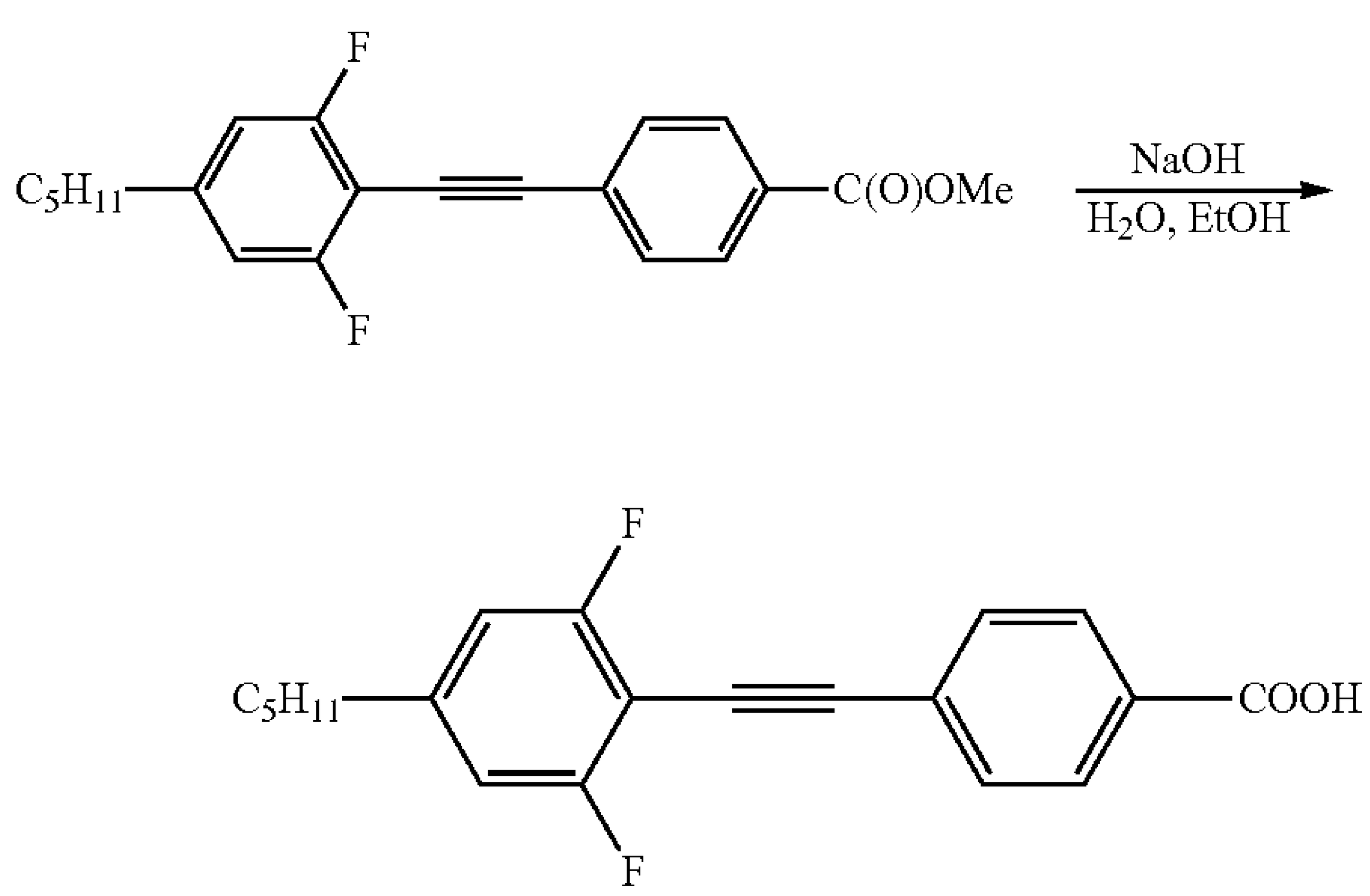
The resulting brown product (19.68 g; 75 mmol) was added into 100 ml of a solvent containing dichloromethane: methanol=1:1 and the resulting solution was stirred until the solid was dissolved. Then, K_2CO_3 (12.16 g; 88 mmol) was added into the solution and the resulting solution was stirred for 4 hrs. After the reaction, dichloromethane and water were used to extract the product, and a product of a yellow liquid in an organic layer was then obtained. The reaction can be expressed by the following equation:



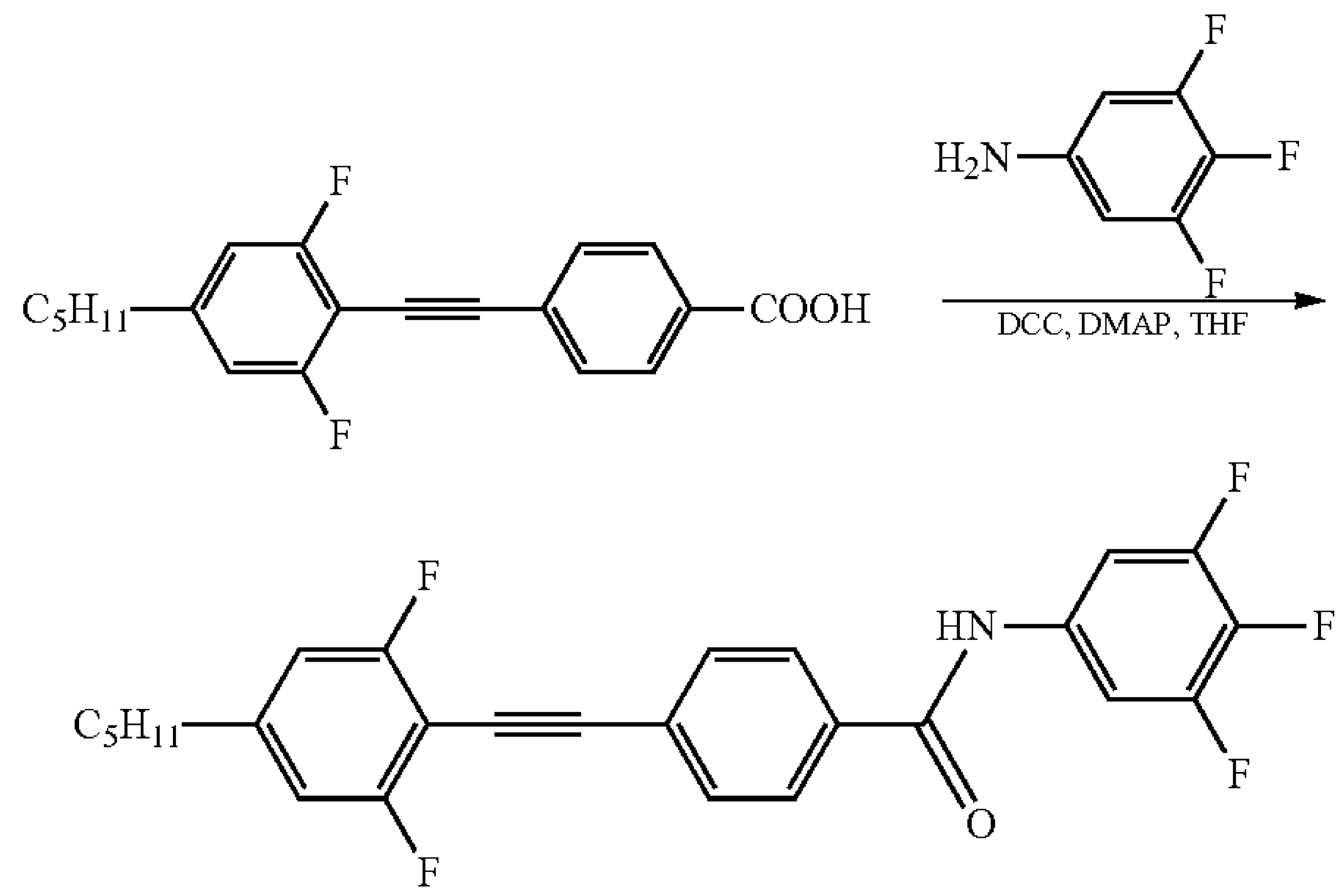
The resulting yellow liquid (17.12 g; 70 mmol), dried triethylamine (60 ml), and dried THF (60 ml) were added into a reaction flask under N_2 atmosphere. Bis(triphenylphosphine)palladium dichloride (0.51 g; 0.7 mmol) and copper iodide (0.14 g; 0.7 mmol) were then added into the flask, and the mixture was stirred for 0.5 hrs. Then, methyl 4-iodobenzoate (19.6 g; 75 mmol) was added into the flask and the resulting solution was heated to 70° C. The reaction continued for 12 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a yellow solid product. The reaction can be expressed by the following equation:



The resulting yellow product was then dissolved in a solution of water: ethanol=1:1 (60 ml), and NaOH (3.6 g; 150 mmol) was added into the solution. The solution was then heated to 60° C. The reaction was continued for 4 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a white solid product. The reaction can be expressed by the following equation:

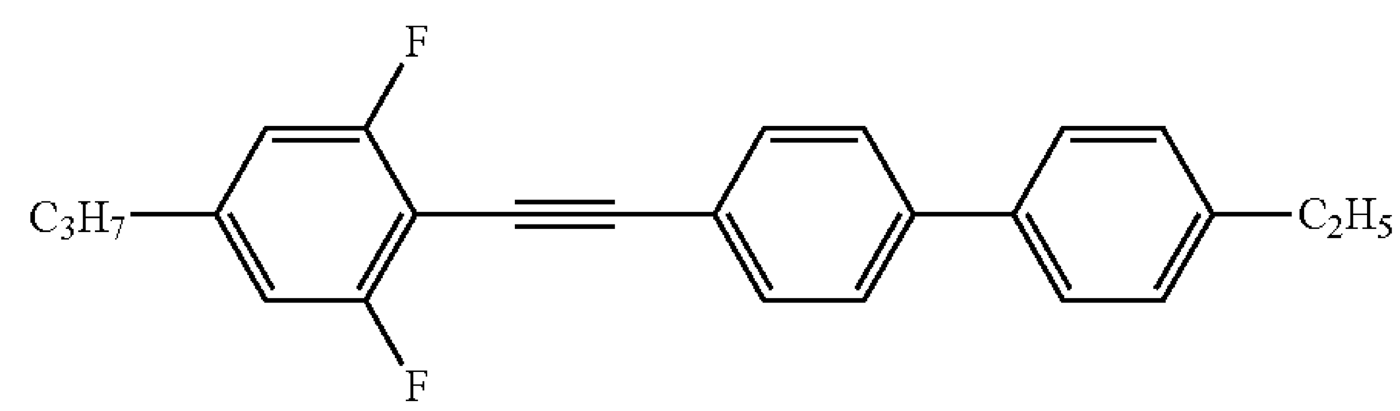


The resulting white product (19.7 g; 60 mmol) and dried THF (50 ml) were added into a flask. After the white product was dissolved, 3, 4, 5,-trifluorophenol, as a white solid, (9.3 g; 60 mmol), 4-(dimethylamino) pyridine (DMPA; 2.9 g; 24 mmol), and dicyclohexylcarbodiimide (DCC; 14.8 g; 72 mmol) were added into the solution under N_2 atmosphere. The solution was then heated to 70° C. The reaction continued for 6 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure. A yellow solid product was then obtained as a crude product. The crude product was recrystallized twice by hexane and dichloromethane to obtain a liquid crystal compound 17 as a white solid (20.1 g; 44 mmol; yield: 44%). The reaction can be expressed by the following equation:



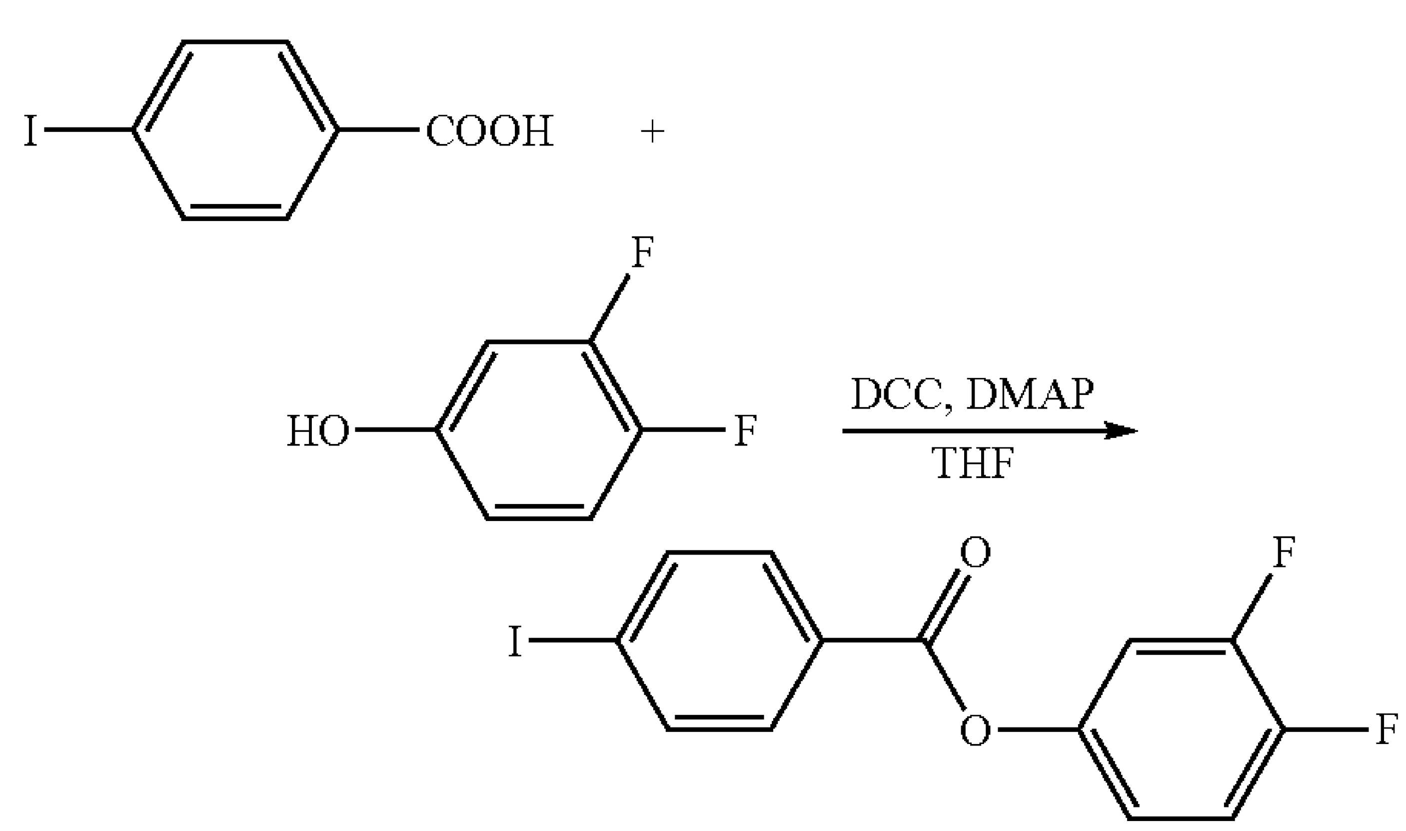
Comparative Example 1

A commercial liquid crystal compound having following formula (purchased from Merck; PPTUI-3-2) was used as the comparative example 1.



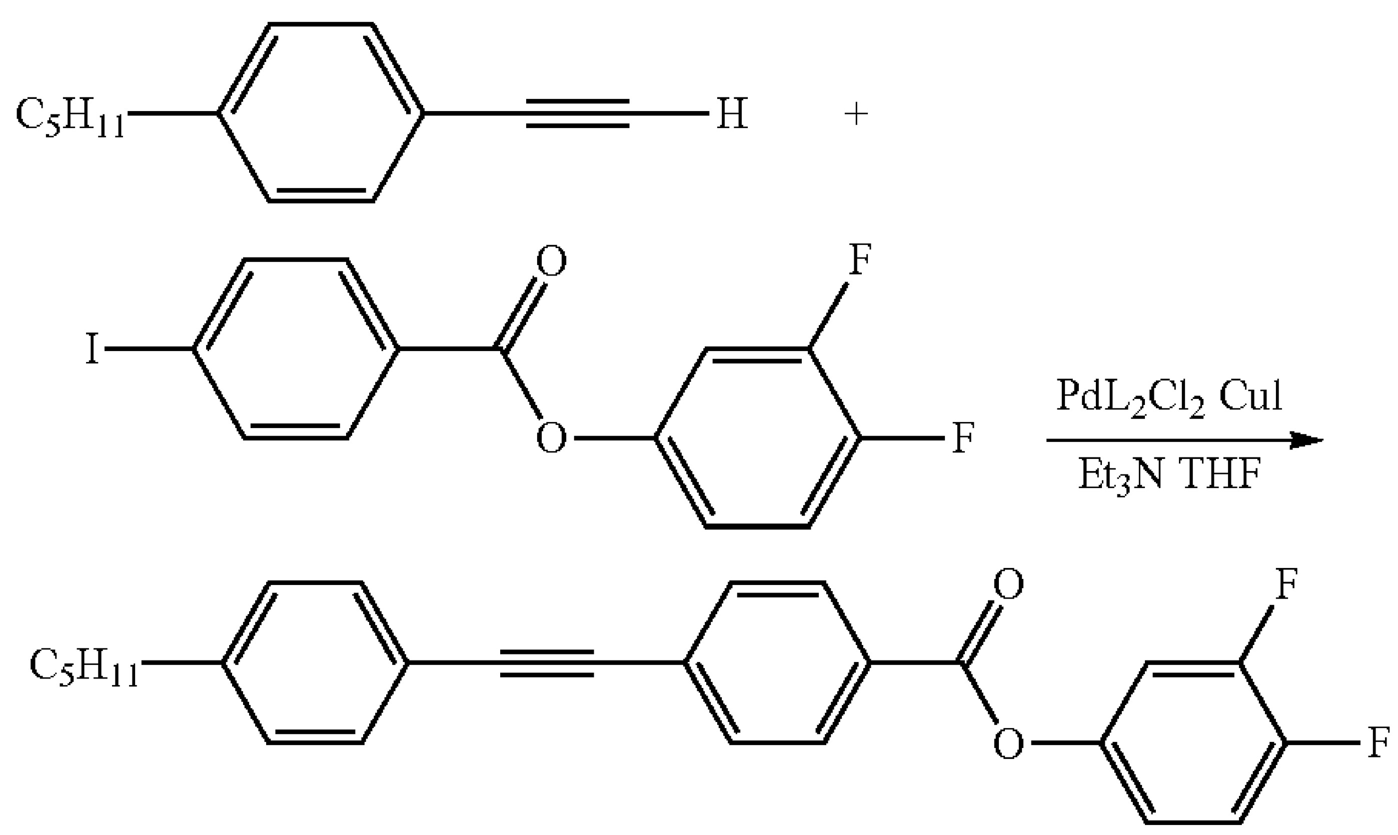
Comparative Example 2

4-Iodobenzoic acid (24.8 g; 100 mmol) and dried THF (60 ml) were added into a flask, and the 4-Iodobenzoic acid was dissolved. Under N_2 atmosphere, 3,4-difluorophenol (14.6 g; 60 mmol), 4-(dimethylamino)pyridine (14.6 g; 60 mmol), and dicyclohexylcarbodiimide (24.6 g; 120 mmol) were also added into the flask. The solution was heated to 70° C., and the reaction continued for 6 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure to obtain a yellow solid product. The reaction can be expressed by the following equation:



Next, the resulting yellow product (32.13 g; 85 mmol), dried triethylamine (60 ml), and dried THF (60 ml) were added into a reaction flask under N_2 atmosphere. Then, bis (triphenylphosphine)palladium dichloride used as a catalyst

(0.51 g; 0.7 mmol) and copper iodide (0.18 g; 0.7 mmol) were added into the flask and stirred for 0.5 hrs. Then, methyl 4-iodobenzoate (15.49 g; 90 mmol) was then added into the mixture. The solution was then heated to 70° C. and the reaction continued for 12 hrs. After the reaction, ethyl acetate and water were used to extract the product, and the resulting organic layer was concentrated under reduced pressure. A yellow solid was then obtained as a crude product. The crude product was recrystallized twice by hexane and dichloromethane to obtain a white solid (28.3 g; 67 mmol; yield: 67%). The reaction can be expressed by the following equation:



Example 5

Dielectric Anisotropy of Liquid Crystal Compounds

Various liquid crystal compounds were added into a passive matrix (PM) liquid crystal formulation or active matrix (AM) liquid crystal formulation respectively to analyze their dielectric anisotropy. A composition of the active matrix (AM) liquid crystal formulation (JM-2069-054) is shown in Table 2.

TABLE 2

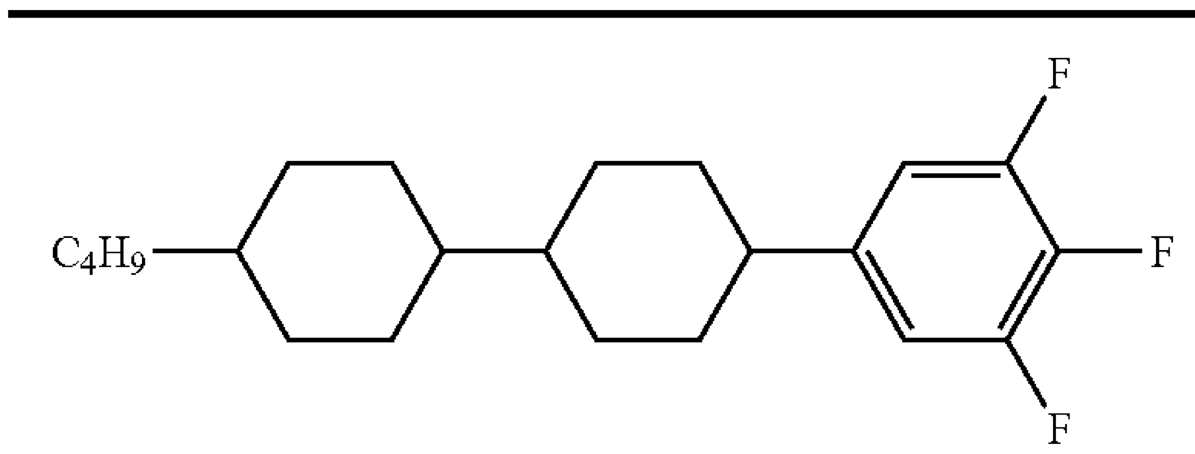
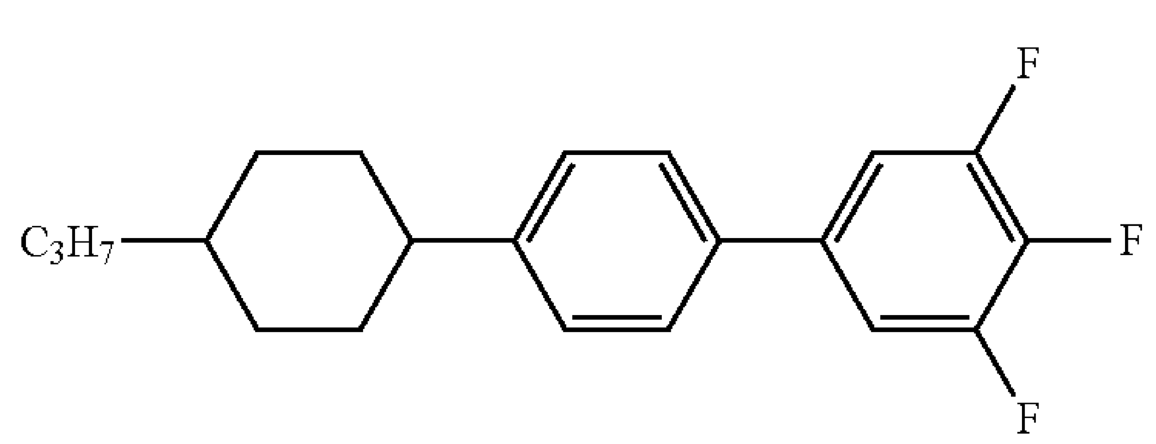
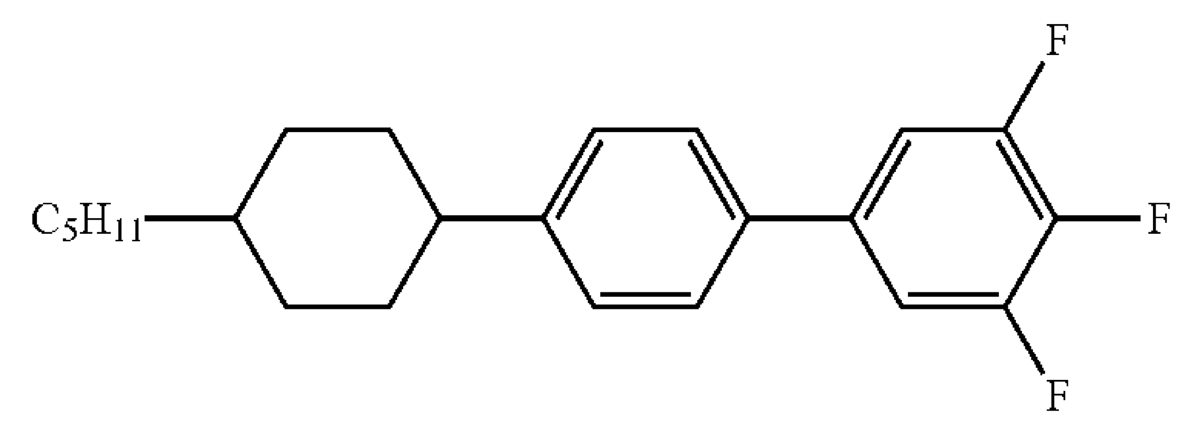
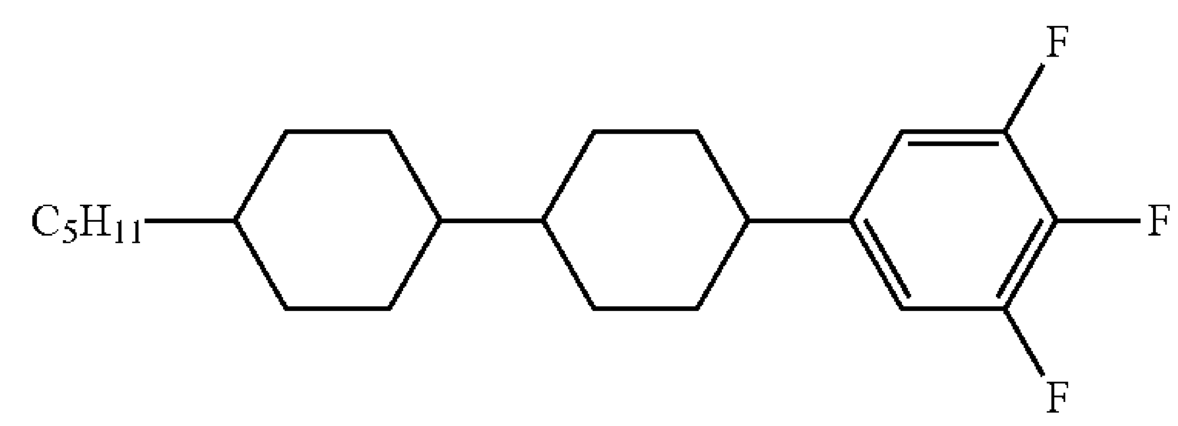
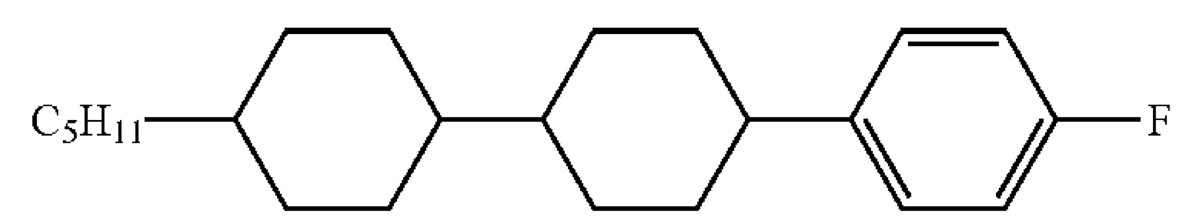
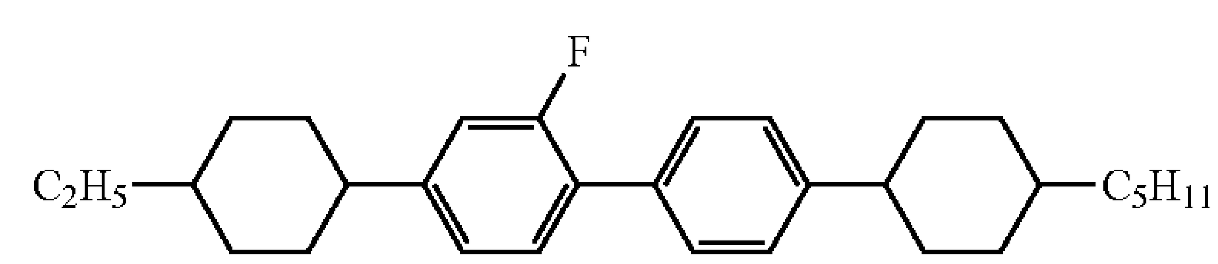
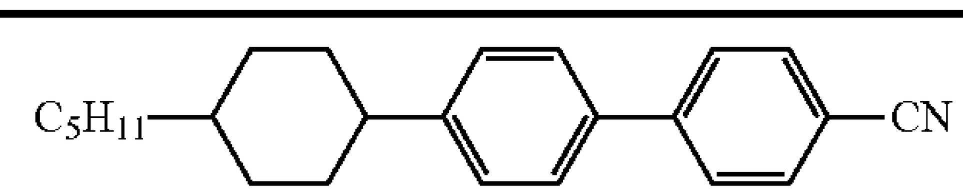
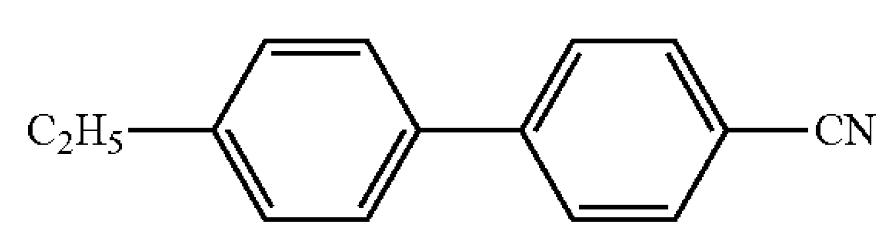
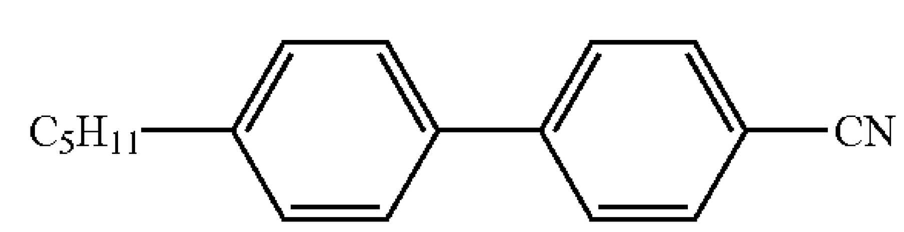
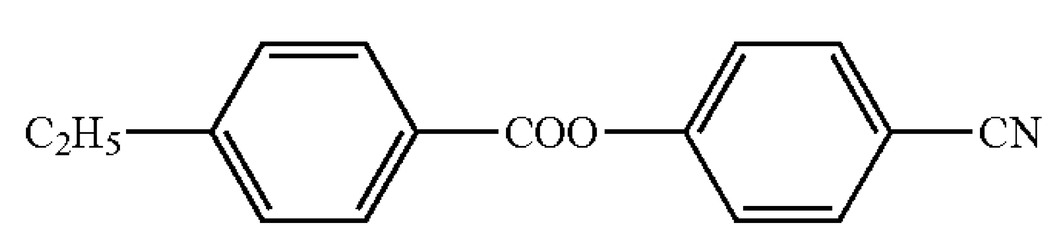
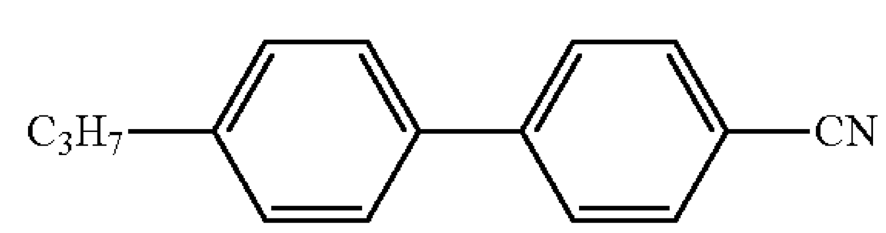
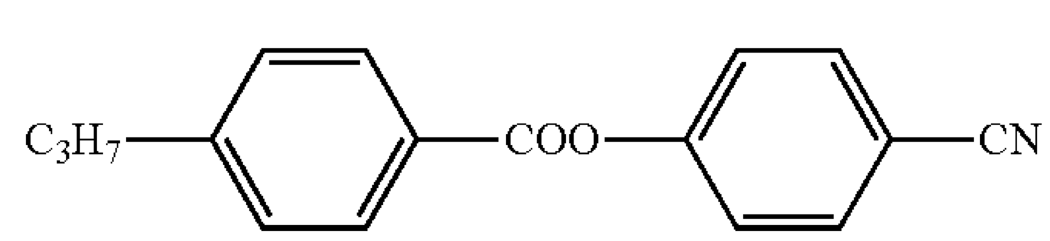
Active liquid crystal formulation (JM-2069-054)	
Liquid crystal monomer	Concentration (wt %)
	11 wt %
	43 wt %

TABLE 2-continued

Active liquid crystal formulation (JM-2069-054)	
Liquid crystal monomer	Concentration (wt %)
	24 wt %
	11 wt %
	4 wt %
	5 wt %

In addition, a composition of the passive matrix (PM) liquid crystal formulation (IBL-087c) is shown in Table 3.

TABLE 3

Passive liquid crystal formulation (IBL-087c)	
Monomer	Concentration (wt %)
	15 wt %
	14 wt %
	34 wt %
	13 wt %
	15 wt %
	10 wt %

The liquid crystal compounds were added into a passive matrix (PM) liquid crystal formulation or active matrix (AM) liquid crystal formulation respectively, wherein each liquid crystal formulation contained 10 wt % of the liquid crystal compound. A refractive index detector (DR-M2) was used to detect the birefringence. A Liquid Crystal Analysis System (LCAS-1) was used to detect the dielectric anisotropy and calculate the birefringence (Δn) and dielectric anisotropy (Δ∈) of each liquid crystal compound. Furthermore, a Differential Scanning calorimetry (DSC) was also used to detect the melting point (T_c), and a Viscometer (CAP1000L) was used to detect the viscosity (η). Table 4 shows the features of the liquid crystal formulation after adding different liquid crystal compounds. In addition, Table 5 shows the dielectric anisotropy (Δ∈) of each liquid crystal compound calculated by LCAS-1.

TABLE 4

Liquid crystal compounds in the liquid crystal formulation

	Δn	Δε	Increase of Δε	T_c (° C.)	η (at 20° C.)
LC (PM)	0.24	17.8	—	97.6	48
LC(PM) + Example 1	0.22	21.2	19.1%	90.1	55
LC(PM) + Example 2	0.22	22.5	26.4%	92.7	57
LC(PM) + Example 3	0.22	22.6	26.9%	92.6	58
LC(PM) + Example 4	0.22	22.1	24.1%	94.3	62
LC(PM) + Comparative example 1	0.24	18.6	4.5%	100.3	45
LC(PM) + Comparative example 2	0.22	18.9	6.2%	97.2	50
LC (AM)	0.15	12.5	—	99.4	37
LC(AM) + Example 1	0.16	17.3	38.4%	95.3	45
LC(AM) + Example 2	0.16	19.4	55.2%	97.9	49
LC(AM) + Example 3	0.16	19.6	56.8%	97.5	49
LC(AM) + Example 4	0.16	19.0	52.0%	98.7	52
LC(AM) + Comparative example 1	0.17	13.9	11.2%	109.7	51
LC(AM) + Comparative example 2	0.16	14.7	17.6%	103.3	45

TABLE 5

Dielectric anisotropy of liquid crystal compounds

	Example 1 (PM)	Example 2 (PM)	Example 3 (PM)	Example 4 (PM)	Comparative example 1 (PM)	Comparative example 2 (PM)
Δε	52	65	66	61	26	29
	Example 1 (AM)	Example 2 (AM)	Example 3 (AM)	Example 4 (AM)	Comparative example 1 (AM)	Comparative example 2 (AM)
Δε	60	82	83	77	27	35

Referring to Table 5, although the structures of the compounds in the comparative examples 1 and 2 were similar to the structures in examples 1-4, the dielectric anisotropy of the compounds in the comparative examples 1 and 2 were both quite low. Therefore, when the compounds in the comparative examples 1 or 2 was added into the active or passive liquid crystal formulations, the dielectric anisotropy of the entire liquid crystal formulation only increased a little. That is, if the compound in the comparative examples 1 or 2 is used in a liquid crystal display, the driving voltage of the display may not decrease effectively.

On the contrary, all the compounds in the examples 1-4 had high dielectric anisotropy. Therefore, when the compounds in the examples 1-4 was added into the active or passive liquid crystal formulations respectively, the dielectric anisotropy of the entire liquid crystal formulation increased markedly. That is, if the compounds in the examples 1-4 are used in a liquid crystal display, the driving voltage of the display may decrease effectively.

Example 6

Additive Amount of the Liquid Crystal Compound 1

Table 6 shows the result of adding different amounts of the liquid crystal compound 1 (example 1) to the active or passive liquid crystal formulation. Table 7 shows the dielectric anisotropy of the liquid crystal compound 1 (example 1) calculated by LCAS-1. The active or passive liquid crystal formulation respectively contains 5 wt %, 10 wt %, or 15 wt % of the liquid crystal compound 1 (example 1).

TABLE 6

Liquid crystal compound 1 in liquid crystal formulation

	Δn	Δε	Increment of Δε	T_c (° C.)	η (at 20° C.)
LC (PM)	0.24	17.8	—	97.6	48
LC(PM) + Example 1 (5 wt %)	0.22	19.2	7.8%	91.8	50
LC(PM) + Example 1 (10 wt %)	0.22	21.2	19.7%	90.1	55
LC(PM) + Example 1 (15 wt %)	0.23	22.9	28.6%	88.9	61
LC (AM)	0.15	12.5	—	99.4	37
LC(AM) + Example 1 (5 wt %)	0.15	14.7	17.6%	96.9	43
LC(AM) + Example 1 (10 wt %)	0.16	17.3	38.4%	95.3	45
LC(AM) + Example 1 (15 wt %)	0.16	19.2	52.8%	94.2	50

TABLE 7

Dielectric anisotropy of liquid crystal compound 1

Sample	Example 1 (PM) 5 wt %	Example 1 (PM) 10 wt %	Example 1 (PM) 15 wt %	Example 1 (AM) 5 wt %	Example 1 (AM) 10 wt %	Example 1 (AM) 15 wt %
Δε	46	52	52	56	60	56

Referring to Table 7, the liquid crystal compound 1 (example 1) had good dielectric anisotropy and solubility for both of the active and passive liquid crystal formulations. In addition, when the additive amount of the liquid crystal compound 1 increased, the dielectric anisotropy of the entire liquid crystal formulation increased markedly.

Example 7

Additive Amount of the Liquid Crystal Compound 2

Table 8 shows the result of adding different amounts of the liquid crystal compound 2 (example 2) to the active or passive liquid crystal formulation. Table 9 shows the dielectric anisotropy of the liquid crystal compound 2 (example 2) calculated by LCAS-1. The active or passive liquid crystal formulation respectively contains 5 wt %, 10 wt %, or 15 wt % of the liquid crystal compound 2 (example 2).

TABLE 8

Liquid crystal compound 2 in liquid crystal formulation

	Δn	Δε	Increment of Δε	T_c (° C.)	η (at 20° C.)
LC (PM)	0.24	17.8	—	97.6	48
LC(PM) + Example 2 (5 wt %)	0.22	20.1	12.9%	94.3	51

TABLE 8-continued

Liquid crystal compound 2 in liquid crystal formulation

	Δn	Δϵ	Increment of Δϵ	T_c (° C.)	η (at 20° C.)
LC(PM) + Example 2 (10 wt %)	0.22	22.5	26.4%	92.7	57
LC(PM) + Example 2 (15 wt %)	0.23	24.5	37.6%	90.2	65
LC (AM)	0.15	12.5	—	99.4	37
LC(AM) + Example 2 (5 wt %)	0.15	15.8	26.4%	98.5	42
LC(AM) + Example 2 (10 wt %)	0.16	19.4	55.2%	97.9	49
LC(AM) + Example 2 (15 wt %)	0.16	22.6	80.8%	97.4	57

TABLE 9

Dielectric anisotropy of liquid crystal compound 2

Sample	Example 2 (PM) 5 wt %	Example 2 (PM) 10 wt %	Example 2 (PM) 15 wt %	Example 2 (AM) 5 wt %	Example 2 (AM) 10 wt %	Example 2 (AM) 15 wt %
Δϵ	62	65	62	80	82	80

Referring to Table 9, the liquid crystal compound 2 (example 2) had good dielectric anisotropy and solubility for both of the active and passive liquid crystal formulations. In addition, when the additive amount of the liquid crystal compound 2 increased, the dielectric anisotropy of the entire liquid crystal formulation increased markedly.

Furthermore, Tables 10 and 11 shows the dielectric anisotropy of liquid crystal compounds in the examples 1-4 and comparative examples 1-2. As shown in Table 10, the liquid crystal compounds in the examples 1-4 had higher dielectric anisotropy, wherein the passive liquid crystal formulation contained 5 wt %, 10 wt %, and 15 wt % of the liquid crystal compound respectively. As shown in Table 11, the liquid crystal compounds in the examples 1-4 had higher dielectric anisotropy, wherein the active liquid crystal formulation contained 5 wt %, 10 wt %, and 15 wt % of the liquid crystal compound respectively.

TABLE 10

Dielectric anisotropy of liquid crystal compounds at various concentration in the passive liquid crystal formulation

	Example 1			Comparative example 1			Comparative example 2		
Conc.	5 wt %	10 wt %	15 wt %	5 wt %	10 wt %	15 wt %	5 wt %	10 wt %	15 wt %
Δϵ	19.2	21.2	22.9	18.2	18.6	18.9	18.6	18.9	19.8

TABLE 11

Dielectric anisotropy of liquid crystal compounds at various concentration in the active liquid crystal formulation

	Example 1			Comparative example 1			Comparative example 2		
Conc.	5 wt %	10 wt %	15 wt %	5 wt %	10 wt %	15 wt %	5 wt %	10 wt %	15 wt %
Δϵ	14.7	17.3	19.2	13.6	13.9	16.0	14.1	14.7	16.4

Example 9

Driving Voltage

Liquid crystal compounds in the examples 1-2 and comparative examples 1-2 were added into the passive liquid crystal formulation (IBL-087c) and active liquid crystal formulation (JM-2069-054) to form liquid crystal displays. The driving voltages of the liquid crystal displays were measured (Table 12).

TABLE 12

Driving voltage of the liquid crystal displays

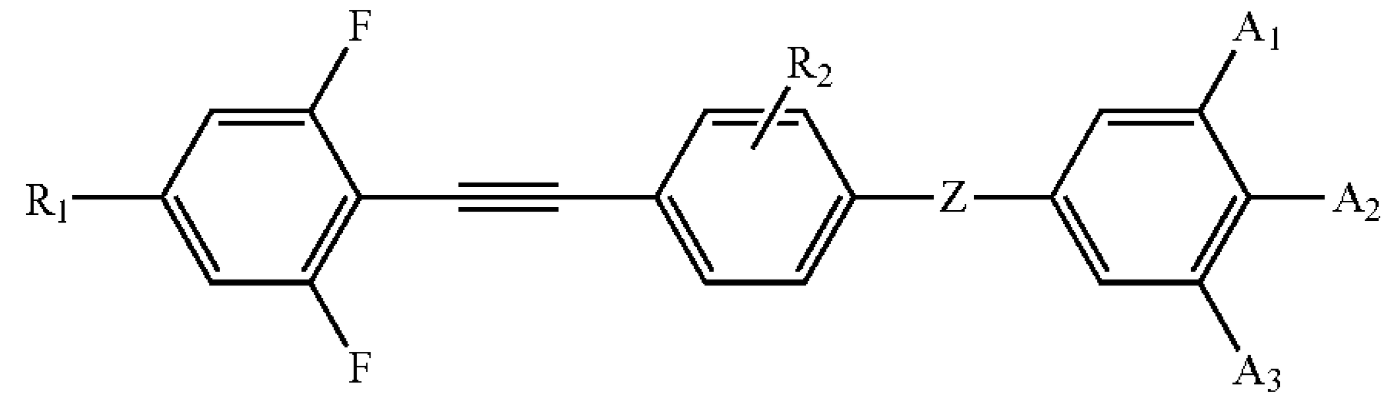
	Conc. (wt %)	Δϵ of liquid crystal compound	Driving voltage (Vth)	Decrease of driving voltage (%)
LC (PM)	—	—	1.22	—
LC(PM) + example 1	15 wt %	52	0.98	16.3%
LC(PM) + example 2	15 wt %	62	0.94	18.6%
LC(PM) + comparative example 1	15 wt %	29	1.13	7.5%
LC(PM) + comparative example 2	15 wt %	35	1.12	8.3%
LC (AM)	—	—	1.65	—
LC(AM) + example 1	15 wt %	56	1.15	25.7%
LC(AM) + example 2	15 wt %	79	1.09	28.1%
LC(AM) + comparative example 1	15 wt %	35	1.46	11.5%
LC(PM) + comparative example 2	15 wt %	38	1.38	16.3%

As shown in Table 12, when the liquid crystal compounds 1 and 2 (examples 1 and 2) were used in the liquid crystal displays respectively, the driving voltages of the liquid crystal displays decreased effectively. However, conventional liquid crystal compounds as in comparative examples 1 and 2 could not effectively decrease the driving voltage of the liquid crystal displays.

While the invention has been described by way of example and in terms of the preferred embodiments, it is to be understood that the invention is not limited to the disclosed embodiments. To the contrary, it is intended to cover various modifications and similar arrangements (as would be apparent to those skilled in the art). Therefore, the scope of the appended claims should be accorded the broadest interpretation so as to encompass all such modifications and similar arrangements.

What is claimed is:

1. A liquid crystal compound having the following formula:



wherein

A_1, A_2, and A_3 are independently hydrogen, halogen, cyano, thiocyanato, or —OCF_3;

R_1 is hydrogen, halogen, C_1-C_{12} alkyl, C_1-C_{12} alkoxy, C_1-C_{12} haloalkyl, C_2-C_{12} alkenyl, or C_2-C_{12} alkynyl;

R_2 is hydrogen, halogen, C_1-C_6 alkyl, C_1-C_6 haloalkyl, cyano, or —OCF_3; and

Z is —O—, —CH_2O—, —C(O)O—, —OCO—, —C(O)NH—, or —CH═CH.

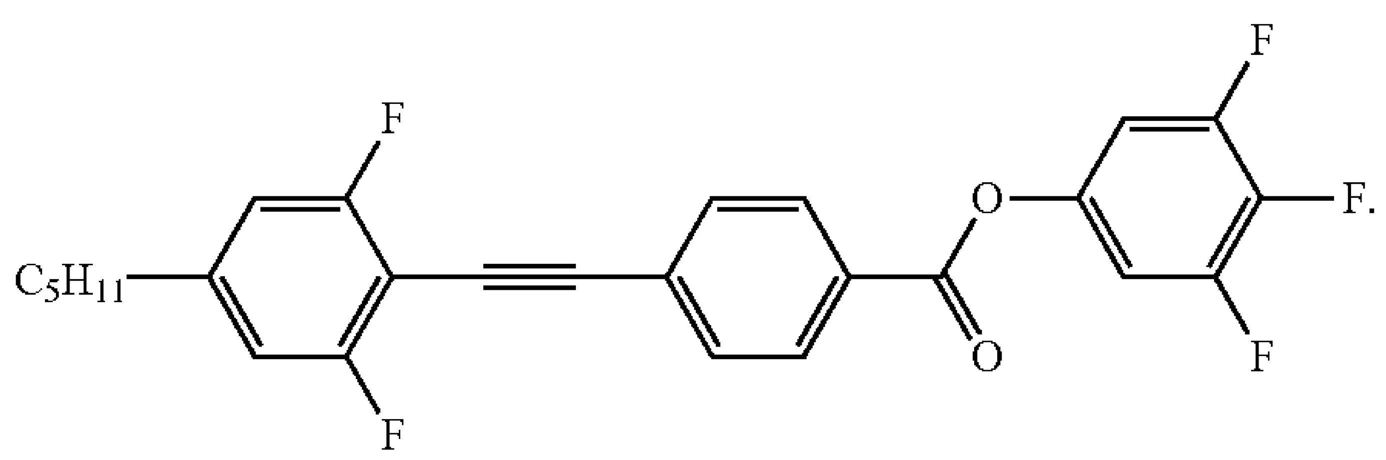
2. The liquid crystal compound as claimed in claim 1, wherein A_1, A_2, and A_3 are independently halogen or cyano.

3. The liquid crystal compound as claimed in claim 1, wherein R_1 is C_1-C_{12} alkyl or C_1-C_{12} alkoxy.

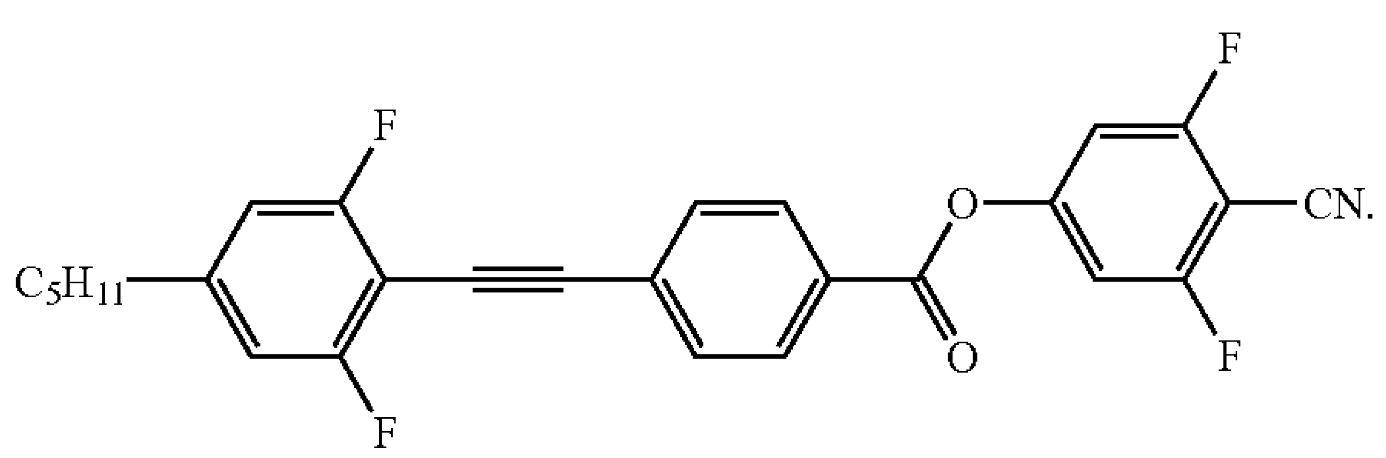
4. The liquid crystal compound as claimed in claim 1, wherein R_2 is hydrogen.

5. The liquid crystal compound as claimed in claim 1, wherein Z is —C(O)O— or —C(O)NH—.

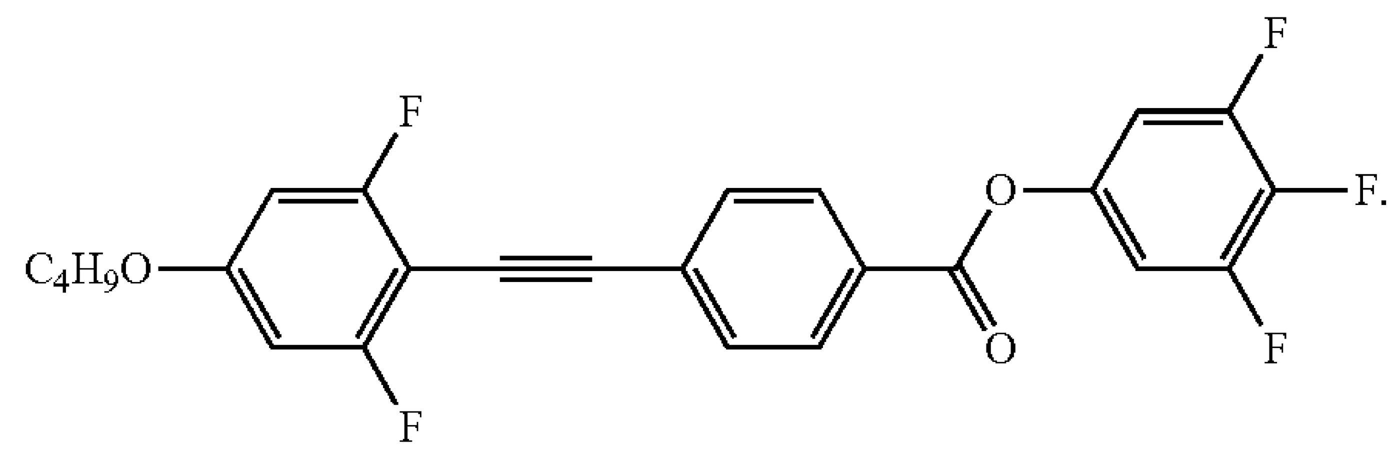
6. The liquid crystal compound as claimed in claim 1, wherein the liquid crystal compound has a following frmula:



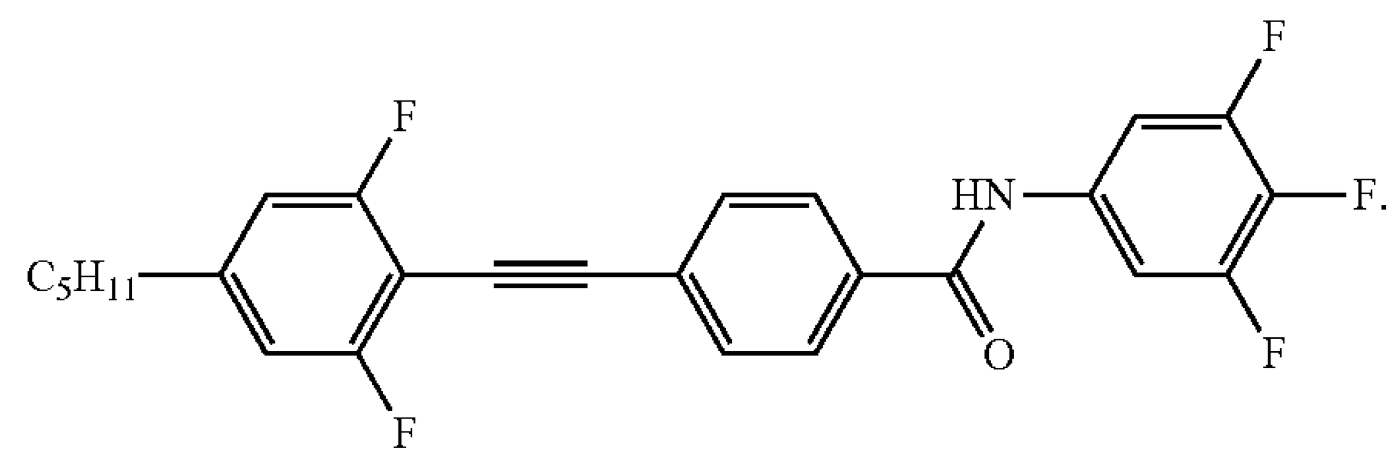
7. The liquid crystal compound as claimed in claim 1, wherein the liquid crystal compound has a following formula:



8. The liquid crystal compound as claimed in claim 1, wherein the liquid crystal compound has a following formula:



9. The liquid crystal compound as claimed in claim 1, wherein the liquid crystal compound has a following formula:



10. The liquid crystal compound as claimed in claim 1, wherein a dielectric anisotropy (Δ∈) of the liquid crystal compound is larger than 45.

11. The liquid crystal compound as claimed in claim 10, wherein the dielectric anisotropy (Δ∈) of the liquid crystal compound is between 45 and 85.

12. A liquid crystal display, comprising:

a first substrate;

a second substrate disposed opposite to the first substrate; and

a liquid crystal layer disposed between the first substrate and the second substrate, wherein the liquid crystal layer comprises the liquid crystal compound as claimed in claim 1.

13. The liquid crystal display as claimed in claim 12, wherein the liquid crystal layer contains 5% to 15% by weight of the liquid crystal compound.

* * * * *

UNITED STATES PATENT AND TRADEMARK OFFICE

CERTIFICATE OF CORRECTION

PATENT NO. : 8,486,497 B2
APPLICATION NO. : 13/340257
DATED : July 16, 2013
INVENTOR(S) : Jian-Wen Lin et al.

It is certified that error appears in the above-identified patent and that said Letters Patent is hereby corrected as shown below:

ON THE TITLE PAGE:

At item (75), Inventors, change "**Chun-Ming Wei**, Banqiao (TW)" to --**Chun-Ming Wu**, Banqiao (TW)--.

Signed and Sealed this
Twenty-second Day of October, 2013

Teresa Stanek Rea
Deputy Director of the United States Patent and Trademark Office